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REPORT

AIR QUALITY SURVEYS IN
UPPER OTTAWA STREET LANDFILL SITE

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EXECUTIVE SUMMARY

The SCIEX TAGA™ 3000 mobile laboratory was used to survey the air quality of the Upper Ottawa Street landfill site, Hamilton, Ontario. Ambient air samples and direct underground vapour samples were obtained and analyzed continuously during August 19, 20, 21 and November 5, 1981. A total number of nine vents and six residential sites were extensively analyzed.

The overall objectives of the program were:

- (a) To qualitatively identify as many pollutants as possible within the vents and in the vicinity of the site. Tables 4.2-1, 4.2-2, 4.3-1 and 4.3-2 show a detailed list of the chemicals identified within the vent vapour phase (Tables 4.2-1 and 4.3-1) and in the residential areas (Tables 4.2-2 and 4.3-2).
- (b) To compare the "air quality" on the landfill to that upwind and downwind of it Table 1-1 shows the various chemicals detected at both the landfill site and the residential sites. This list shows the chemicals believed to originate from the landfill site during the study period. It is to be emphasized that other chemicals detected within the boundaries of the landfill may also be in the residential areas at concentrations below the detection limits of the TAGA™ 3000 system.

The results in Table 1-1 indicate a consistent trend in that chemicals observed within the vents are also observed on site 5, Arbur Street. This location was upwind of the site and hence was considered a background site. This trend indicates transport of the chemicals underground and surfacing in the area of Arbur Street. Subsequent to our Draft Report we learned of supporting evidence for this observation from the Landfill Study Group. It is thought that the underground water movement is in the direction of Arbur Street and that a sewer system for the Municipality is also located in that area.

Based upon the extensive results, the complexity of the detected chemicals and their potential effects, we recommend that:

- (a) Retro-calibration of a select number of chemicals be performed to estimate their concentration within an order of magnitude.
- (b) Quantitative measurements be conducted on site in order to determine the levels of "worst case" chemicals.

In order to choose twenty chemicals for further study, a procedure or criteria for selection has to be developed. It was agreed between SCIEX™ and the Study Group, that a comprehensive background tabulation be conducted where the uses, toxicity and Threshold Limit Values (TLV) for detected chemicals be used. The available information is given in Appendix 2.

TABLE 1-1

Tentative Assignment of
Unusual Chemicals Jointly Found At
Residential Sites and Landfill Vents. The sites indicate:

Tekawitha School	= Site 1
10 Meters from Gate	= Site 2
Lime Ridge Road	= Site 3
Church Stone & Upper Ottawa	= Site 4
Arbur Street	= Site 5

Chemical	Sites	Vents
(A) Positive Mode		
Methoxyamine	5	1,2,2A
Acrolein	3	1,2,2B,4A,4B
Ethylmethyl Ether/ propyl alcohol/ methyl formate	2,5	0
Butane nitrile	2	2,2A
Crotonaldehyde/ methyl vinyl ketone	5	1,2,2A
Methyl cellosolve/ propyleneglycol trimethyleneglycol	3,5	2
Dimethyl sulfoxide/ 2-mercaptoethanol	3	3,4A
Pyrazine/pyridazine/ pyrimidine	5	1,2,4A
Methylacrylate	2,3,5	2
Aminopyridine/phenol	1,2,5	3,4,2B
Furfural/1-pentol/ methanesulfonic acid	1,3,5	1,2,3,4,2A,4A,0
Cyclohexanone/lactone/ maleic anhydride	2,5	1,2,4,2A,2B,4A
Cresols/quinone	5	1,2
Aminophenol	1	2,2A,2B,4A,0
Hydroquinone	1,2,3,5	1,2,3,4,2A,2B,4A,4B,0
Maleic hydrazide/triethylenediamine sorbic acid/cycloheptanone/	5	2,2B,4A

Chemical	Sites	Vents
2-Heptanone	5	2,2B,4A
Heptanol/butylacetate	1,3,5	2,4,2B
3-Sulfolene/benzofuran/ cellosolve	3	2,3,2B
Xylenol/benzoic acid/ phenethylalcohol	5	1,2,4,0
Melamine/pyrogallol	2,3,5	2,2B
N-Butyl acrylate/ethylamylketone hexylmethyl ketone	3	2,2B,4A
C ₂ -Cresols/nitro anilines/ 2-(ethylsulfonyl) ethanol	1,5	1,2,2A,2B,4A,4B,0
Fumaric acid, dimethyl ester/ naphthol	3,5	2B,4A
Acetaminophen	2	2A,2B
Citronellol/menthol/ rhodinol	1,3	4,2B,4B
2-Nitro-2-propyl-1,3-propanediol	1,2	3,4,2B
Dehydroacetic acid	3	2,2A,2B
2-Phenoxyethanol acetate	3,5	2,2A,2B
1-Naphthol isothiocyanate	2	2,4
Salicylanilide	1	2A,4A
(B) Negative Mode		
Formic acid	1,2	1, 2A, 2B, 4A, 4B
Thiocyanic acid	4	2
Acrylic acid/oxid. prod. of acrolein	5	1,2,4A
Propanoic acid	5	1,2A,2B, 4A
Chloric acid/crotonic acid/ methacrylic acid	4,5	2,2B,4A,4B
Pyruvic acid	1,4,5	1,2,3,2A,2B,4A,4B
Lactic acid	1,2,3,4,5	2,3
Valeric/isovaleric acid	4,5	1,2,2A,2B,4A,4B
Levulinic acid/fumaric acid/ maleic acid/n-caproic acid	1,4,5	1,2,3,4,2A,2B,4B
Chlorinated phenols/ Cyclohexane carboxylic acid	4	1,2,2B,4A,4B

<u>Chemical</u>	<u>Sites</u>	<u>Vents</u>
Heptanoic acid	4	1,2,4B
Caprylic acid	4	1,2,3,4,2A,4B
Pelargonic acid	1	1,3,4

2.0 INTRODUCTION

2.1 General

This report contains the results of surveys conducted at the Upper Ottawa Street Landfill Site (UOSL) and its vicinity.

The overall objectives of the program were:

- (a) To qualitatively identify as many pollutants as possible emanating from the UOSL site.
- (b) To compare the "air quality", in terms of types of pollutants, on the UOSL to air quality upwind and downwind of the site. This will enable the UOSL Study Group to determine whether or not the landfill site is contributing any air pollutants to the general background in Hamilton.

2.2 Tasks

In order to achieve the above objectives, field surveys were conducted on August 19, 20, 21 and November 5, 1981. The sampling program consisted of discrete samples and realtime monitoring on location using the mobile Trace Atmospheric Gas Analyzer (TAGA™ 3000). Discrete samples were collected as follows:

- (a) gas badges from vents 1 and 2 (Dupont: Pro-Tech, activated charcoal).
- (b) Florisil cartridges from vents 1 and 2.
- (c) charcoal cartridges from vents 1 and 2.

These samples were submitted to Wellington Environmental Consultants Incorporated of Guelph, Ontario, for processing and analysis using a capillary column gas liquid chromatograph with an electron capture detector (GLC-ECD). Appendix I gives Wellington's brief report.

TABLE 2.2-1
Summary of Sampling Sites and Dates

<u>Date</u>	<u>Location</u>
August 19	Inner Gate of Landfill Site Tekokwitha School Vent #4 (opposite Arbur St.) Vent #3 (opposite Arbur St.) Vent #2 (opposite Stone Church Rd.) Vent #1 (opposite Stone Church Rd.)
August 20	Vent #0 (opposite Ottawa St.) Vent #1 Vent #2
August 21	Lime Ridge Road (Solomone St.) Stone Church & Upper Ottawa St. Arbur St.
November 5	Vent #2A (old solidification site) Vent #2B (old solidification site) Vent #4A (same as 4, new core) Vent #4B (same as 4, new core)

The real time sampling locations are shown in Table 2.2-1. The surveys conducted on November 5, 1981 were restricted to the newly cored vents. The fresh vents 2A and 2B are on site of the old solidification pools, while vents 4A and 4B are a replacement for vent 4 which is thought to be plugged. Figure 2.2-1 shows the approximate locations of the sampling sites.

Air bag samples were collected on November 5, 1981 from vents 4A and 2A for subsequent analysis on a TAGA™ 6000 MS/MS system. Due to the unavailability of the TAGA™ 6000 system, the samples were analyzed on November 16 and 25, 1981 for Vents 4A and 2A respectively.

2.3 Sampling Methodology

The sampling of ambient air, in the TAGA™ system, is performed by a high capacity air pump. The pump draws ambient air into the ionization region at flows of 0.5 to 10 L/sec through 19mm (ID) tubing. During the current surveys, the flow rate was kept at about 1.7 L/sec. The high flow and wide tubing minimize memory effects due to wall absorption for most chemicals. Ambient air samples were obtained at the residential sites and "outside" the vents on site. Direct sampling of gases from within the vent was accomplished by extending the sampling line inlet directly into the vent. This allows the detection of the largest possible number of chemicals since neither "dilution" by mixing with ambient air nor dispersion can occur during sampling.

2.4 Miscellaneous Observations

It is to be noted that during the surveys, Vent #1 was "active". The pipe was too hot to the touch due to extensive exothermic reactions taking place within the site. This was also manifested by condensation at the cooler exposed parts of the pipe due to the temperature differential between the vented gases and ambient conditions.

During August 19, 1981 sampling, Tekokwitha School site was chosen as the downwind location, similarly for the site within UOSL property, 10 meters from inner gate.

August 20 and November 5, 1981 surveys were restricted to direct sampling of vented gases from within the vent tubes and outside the vents.

Monitoring on August 21, 1981 was restricted to residential areas. Both sites on Lime Ridge Rd. (Solomone St.) and Arbur St. were upwind of the UOSL site where as the the Stone Church & Upper Ottawa sampling location were directly downwind of the site.

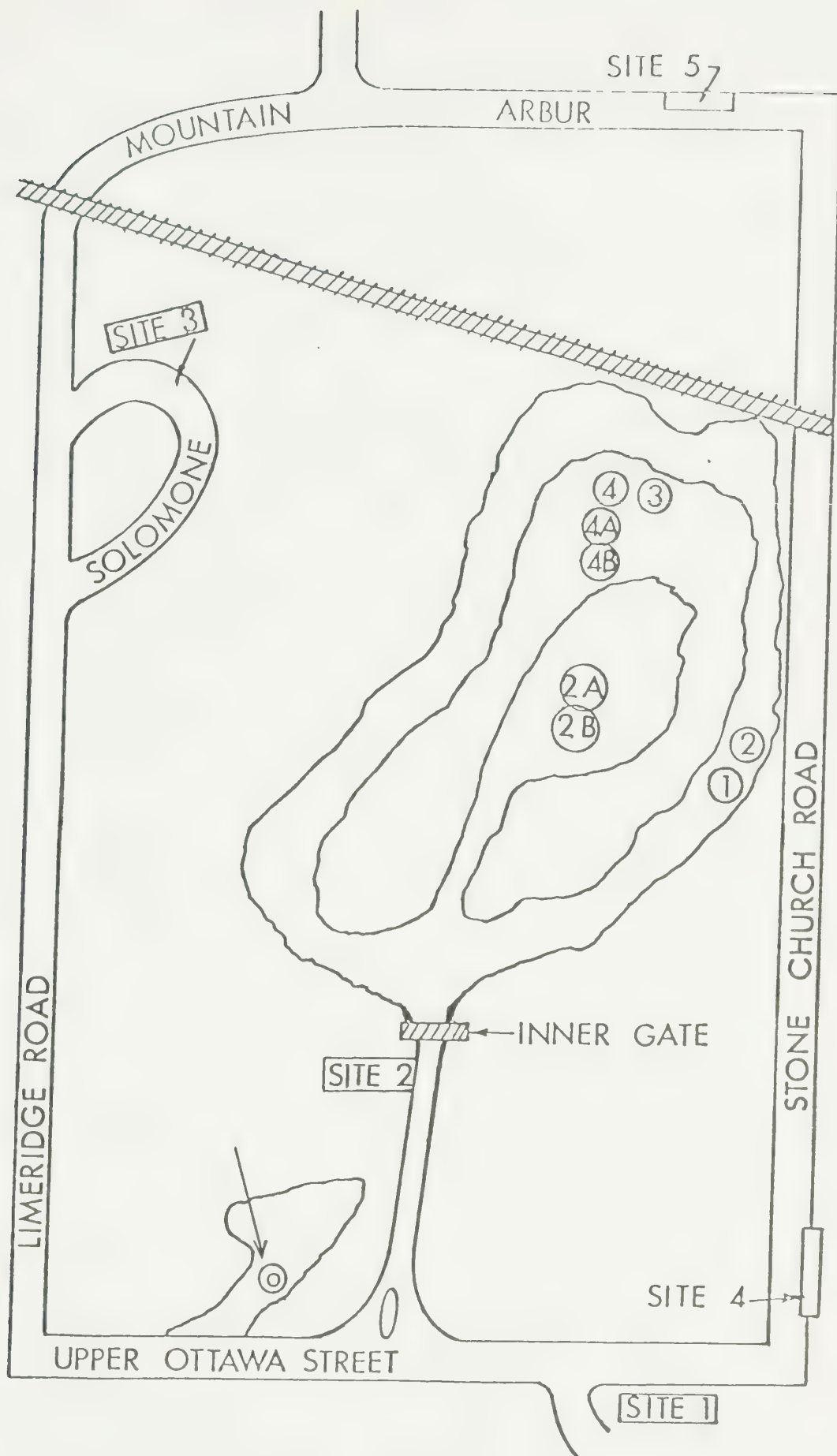


FIGURE 2.2-1 Approximate locations of the sampling sites.

3. ANALYSIS METHODOLOGY

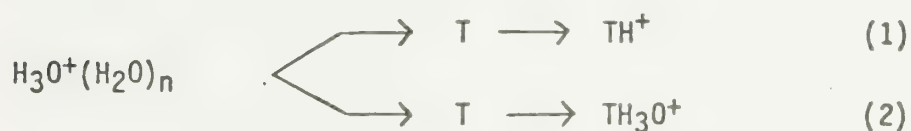
3.1 Introduction

In order to fully comprehend the results and their significance, a brief summary of the TAGA™ methodology is necessary.

3.2 TAGA™ Technology

The TAGA™ technique is based on the use of mass spectrometry to identify and/or quantify trace species in gases at atmospheric or near atmospheric pressure. To make this approach practical for trace concentrations in the range of 1 in 10^6 to 1 in 10^{14} , it is necessary to produce a massive degree of pre-separation or pre-selection of the trace gas molecules from normal air constituents before their introduction into the mass spectrometer. This is done in Atmospheric Pressure Chemical Ionization (APCI) by an extremely rapid preferential ionization of the trace gas molecules using as reagents the ions produced in a primary ionization process from air. The primary ions are derived from water and oxygen for the positive and the negative modes, respectively.

In the positive mode, the reactant ions are dominated by the series $H_3O^+ (H_2O)_n$ which in turn ionize traces by simple non-fragmenting soft-ionization processes, as:



In the negative mode, the ions $O_2^-(H_2O)_n$, CO_3^- tend to be the dominant species which lead to simple non-fragmenting ionization processes such as:



The symbol T, in all equations, represents a trace constituent in ambient air, carrier reagent gas.

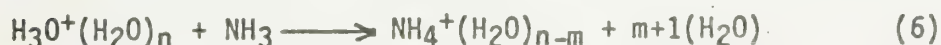
In the positive ion mode, species with the highest gas phase basicity (proton affinity) tend to be the most reactive, while in the

negative ion mode, species with the highest gas phase acidity or electron affinity are the most reactive. Thus the ease of detection of traces will depend upon their relative basicities, acidities, ionization potentials or electron affinities to these primary reactant ions.

The classes of molecules that show high reactivity can be generally classified as those being polar or polarizable. Molecules containing a heteroatom such as O,N,P,S, halogen, a metal etc., and those containing conjugated double bonds fall into this category. Saturated alkanes, unconjugated alkenes, and cyclic hydrocarbons do not show any appreciable reactivity and thus the TAGA™ is "blind" to these chemicals under atmospheric pressure chemical ionization (APCI). A new ionization source developed at SCIEX™ overcomes this shortcoming if operated at reduced pressure (approximately 1 torr). This however, was not used for any of the surveys conducted at UOLS.

3.3 TAGA™ Selectivity

As discussed in the previous section, the classes of compounds that can be detected by the TAGA™ are those containing heteroatoms. This constitutes the first degree of selectivity. A second degree of selectivity depends on the utilization of the fact that reactivities of different chemical classes depend on the relative magnitudes of the thermochemical properties (basicities, acidities, ionization potentials and electron affinities) for the reagent and the trace components. For example, if ammonia is added to the carrier gas in parts per million or greater concentrations, the proton hydrates, $H_3O^+(H_2O)_n$, will rapidly pass a proton to the ammonia forming ammonia hydrates as well as ammonia clusters, reactions (6) and (7) respectively.



Since the basicity (proton affinity) of ammonia is so much higher than that of water, the ammonium ion, NH_4^+ , will protonate fewer types of trace compounds than would the hydronium ion, H_3O^+ . This will effectively "clean" up the spectrum by removing peaks due to oxygenated organics which were protonated by water, and intensify the peaks due to nitrogen based compounds. Thus the use of ammonia is said to "highlight" the nitrogen-containing species as amines, amides, etc.

Table 3.3-1 shows a summary of the chemical ionization reagents used to highlight chemicals of environmental concern. These reagents were used at the UOSL and its vicinity.

3.4 Data Acquisition

The TAGA™ 3000 system can acquire real time data in two generalized modes:

- (a) Targeted compound analysis where the nature of the chemical is known. Thus prior calibration of the TAGA™ is performed and the selected chemicals up to 8 at a time, are monitored as a function of time while stationary or mobile. This mode was not used at UOSL since no prior knowledge of the chemicals was available.
- (b) Scanning mode for unknowns. In this mode, the TAGA™ 3000 is set at a unit mass resolution in the mass-to-charge range of 2 to 500 atomic mass units. This range encompasses most of the volatile chemicals to be expected in ambient air. Because of the variety of chemicals that can have the same nominal mass-to-charge ratio, within 1 amu, a unique and unequivocal identification of a detected peak cannot be guaranteed. However, the use of selective chemical ionization reagents, Table 3.3-1 and "context" as well as tables of thermochemical parameters (proton affinities, ionization potentials, gas phase acidities, and electronegativities) can narrow the number of possible compounds to within two or three chemicals. Further detailed experimentation can be designed, in most cases, to achieve better identification. This limitation was resolved by developing the TAGA™ 6000 MS/MS system.

3.5 Data Reduction

The acquired data at the UOSL site can be reduced in two general approaches:

- (a) an internally consistent single site analysis where the data for each sampling site is analyzed without reference to an upwind or background site. In this case, the data acquired under normal water and oxygen ion chemistries are analyzed and then subtracted from data obtained using other chemical ionization reagents. The resultant information can then be used to obtain a list of chemicals detected on the site.

TABLE 3.3-1

Summary of Chemical Ionization Reagents Used to Highlight
Chemicals of Environmental Concern

<u>Reagent</u>	<u>Highlighted Classes</u>
POSITIVE MODE:	
$\text{H}_3\text{O}(\text{H}_2\text{O})^+_{\text{n}}$	Oxygenated Organics: ketones, alcohols, esters, etc.
NH_4^+	Nitrogen-Containing species: amines, amides, etc.
C_6H_6^+	Aromatics, polyaromatic hydrocarbons
photolysis pre-reactor	Sulfur compounds, alkenes
NEGATIVE MODE:	
$\text{O}_2^-(\text{H}_2\text{O})_{\text{n}}$	Phenolic group, carboxylic acids, aldehydes, SO_2 , NO_2
photolysis pre-reactor	Sulfur compounds (RSH, RSR, RSSR)

- (b) comparative data analysis where two sites are compared regarding their differences and similarities. This allows for background subtraction or correction. For example, two vents can be directly compared by the computer to determine whether there are qualitative or quantitative differences in their contents.

As a first approach, it is usually recommended that data be analyzed according to the internally consistent method, part (a) above. Depending on the results further analysis according to part (b) can then be efficiently and economically utilized. This approach has been adopted in this report.

3.6 Data Interpretation

The peak assignment, or identification is based on several factors as follows:

- (a) Thermochemical parameters: proton affinity, ionization potential, gas phase acidity and electronegativity.
- (b) Reactivity under various chemical ionization reagents and at APCI conditions.
- (c) Context. The Merck Index and the EPA/NIH Mass Spectral data bases were consulted. Each detected peak was matched with all possible chemicals according to the above data base. A process of elimination based on the known behaviour in the TAGA™, (a) and (b) above, was used to arrive at a list of most likely chemicals. This list was further reduced by consulting the Merck Index regarding the uses of each chemical on the short list. Chemicals that were not used in large industrial quantities were eliminated as unlikely to be found in an industrial landfill site. It is to be noted that this is only an assumption to reduce the list of detected chemicals into a more manageable size. It is to be expected that some non-industrial use chemicals will be formed upon interaction of two industrial chemicals landfilled in the same location. As mentioned in Section 2.4, evidence of such interaction was observed in vent #1 during the sampling program.

4.0 RESULTS

4.1 Introduction

Extensive analysis of data for each site was performed as outlined in the previous section. This was followed by grouping the data into two generalized categories: chemicals that are normal constituents of ambient air and those considered unusual. The former group will not be included in this report. The unusual group of chemicals will be presented below.

4.2 Chemicals Detected in the Negative Ion Mode

The final results for this group of chemicals with all relevant information are included in Tables 4.2-1 and 4.2-2. The tables are divided into the following columns; mass-to-charge, M/Z; empirical formulae assignment; comments or identification whenever possible of the responsible chemical; and the sampling locations used in this survey. Table 4.2-1 shows the vents where a given chemical was detected, while Table 4.2-2 shows the same information for the residential sites. In other words, the two tables are identical except for the sampling locations. Table 4.2-1 deals with the vents while Table 4.2-2 shows the residential sites. The two tables can be used to determine whether a detected chemical originates in the UOSL site or is a constituent of the Hamilton urban environment. Chemicals detected on (Stone Church Road and Upper Ottawa Street) but not on Lime Ridge Rd or Arbur St. can most likely be attributed to the UOSL site, and similarly for chemicals detected at Tekokwitha School. It is to be noted that chemicals detected on the UOSL but not in the residential areas are not necessarily absent from the latter; these chemicals may exist at concentrations below the detection limits of the TAGA™ 3000 in realtime.

4.3 Chemicals Detected in the Positive Ion Mode

Similar to the results in Section 4.2, the final list of unusual chemicals detected in the positive ion mode is given in Table 4.3-1 for the vents and in Table 4.3-2 for the residential sites. The self explanatory tables are structured similar to Tables 4.2-1 and 4.2-2 and can be used for the same purposes.

Chemicals Detected in Air Bags

The air bag samples were analyzed on the TAGA™ 6000 MS/MS. Due to the fact that only water ion chemical ionization was used and the unavoidable delay in the analysis, these results are limited in nature. The detected chemicals using the MS/MS system are indicated by a star on the m/z entry in Table 4.3-1.

SUMMARY RESULTS OF CHEMICALS TENTATIVELY IDENTIFIED WITHIN THE VENTS USING THE NEGATIVE ION MASS SPECTRAL ANALYSES.

M/Z	ASSIGNMENTS	COMMENTS	VENT* 0	VENT 1	VENT 2	VENT 2A	VENT 2B	VENT 3	VENT 4	VENT 4A	VI 4
35	35Cl ⁻	possibly from chlorinated organic compounds	ND	x	x	x	x	x	x	x	x
37	37Cl ⁻	possibly from chlorinated organic compounds	ND	x	x	x	x	x	x	x	x
42	CNO ⁻	isocyanyl anion	ND				x				
45	HCDO ⁻	formic acid	ND	x		x	x			x	x
55	C ₃ H ₃ O ⁻	acrolein	ND		x						
57	CNS ⁻	thiocyanic acid	ND		x						
59	C ₂ H ₅ O ₂ ⁻	acetic acid	ND	x							
61	C ₂ H ₅ S ⁻	ethyl mercaptan	ND			x					
69	C ₃ H ₂ O ₂ ⁻	propionic acid	ND			x					
71	C ₃ H ₃ O ₂ ⁻	acrylic acid/Oxid. Prod. of mass 55	ND	x	x						
72	C ₂ H ₂ NS ⁻	methyl thiocyanate	ND								
73	C ₃ H ₅ O ⁻	propanoic acid	ND	x		x	x			x	
75	C ₂ H ₃ OS ⁻ /C ₂ H ₃ O ₃ ⁻	thio acetic acid/glycolic acid	ND		x						
77	C ₂ H ₅ SO ⁻	ethyl sulfonic acid	ND	x	x	x	x				
83	ClO ₃ ⁻ (Cl=35)	chloric acid	ND		x						
85	ClO ₃ ⁻ (Cl=37)/C ₄ H ₅ O ₂ ⁻	chloric acid/crotonic acid or methacrylic acid	ND		x		x			x	
87	C ₃ H ₃ O ₃ ⁻	pyruvic acid	ND	x	x	x	x	x		x	
89	C ₃ H ₆ O ₃ ⁻	lactic acid	ND		x						
91	C ₃ H ₇ SO ⁻	propyl mercaptan derivative	ND			x	x				
92	(C ₂ H ₅ NO ₃) ⁻	ethyl nitrate anion	ND								
93	C ₂ H ₅ SO ₂ ⁻	ethyl mercaptan derivative	ND	x	x	x	x				
93	C ₅ H ₅ O ⁻ /	phenol	ND								
95	C ₄ O ₃ S ⁻	methanesulfonic acid	ND						x		
99	C ₅ H ₇ O ₂ ⁻	carboxylic acid	ND	x	x		x				
101	C ₅ H ₉ O ₂ ⁻	valeric acid or isovaleric acid	ND	x	x	x	x				
105	C ₄ H ₉ SO ⁻	butyl mercaptan derivative	ND			x	x				
107	C ₃ H ₇ SO ₂ ⁻	propyl mercaptan derivative	ND	x							
107	C ₇ H ₉ O ⁻	cresol	ND		x				x		
108	C ₆ H ₆ NO ⁻	nicotiny alcohol	ND			x	x		x	x	
109	C ₂ H ₅ SO ₃ ⁻	ethyl mercaptans derivative	ND		x	x	x				
111	C ₆ H ₇ O ₂ ⁻	sorbic acid	ND		x	x	x				
115	C ₅ H ₇ O ₃ ⁻ /C ₄ H ₃ O ₄ ⁻ /C ₆ H ₁₁ O ₂ ⁻	levulinic acid/fumaric acid or maleic acid/n-caproic acid	ND	x	x	x	x	x	x	x	
121	C ₄ H ₉ SO ₂ ⁻	butylmercaptan or ethyl sulfide	ND	x							
121	C ₆ H ₉ O ⁻ /C ₇ H ₅ O ₂ ⁻	benzoic acid/dimethylphenol	ND		x				x		
122	C ₆ H ₄ NO ₂ ⁻	nitrosophenol or picolinic acid	ND								
123	C ₃ H ₇ SO ₃ ⁻	propyl mercaptan derivative	ND				x				
125	C ₂ H ₅ SO ₄ ⁻	ethyl sulfate or dimethyl sulfate	ND				x				
127	C ₆ H ₄ ClO ⁻ /C ₇ H ₁₁ O ₂ ⁻	chlorinated phenols/cyclohexane carboxylic acid	ND	x	x		x				
129	C ₇ H ₁₃ O ₂ ⁻	heptanoic acid	ND	x	x						
131	C ₇ H ₁₅ S ⁻	hepta mercaptan derivative	ND	x							
135	C ₈ H ₇ O ₂ ⁻	toluic acid or phenylacetic acid	ND		x						
135	C ₅ H ₁₁ SO ₂ ⁻	pentyl mercaptan derivative	ND								
137	C ₄ H ₉ SO ₃ ⁻	butyl mercaptan, ethyl sulfide derivatives	ND								
139	C ₇ H ₄ FO ₂ ⁻ (?)	fluorobenzoic acid(?)	ND		x						
141	C ₆ H ₅ O ₄ ⁻ (?)	kojic acid(?)	ND								
142	C ₆ H ₉ NO ₅ ⁻	NI	ND		x						
143	CH ₃ (CH ₂) ₆ COO ⁻	caprylic acid	ND	x	x	x		x			
153	C ₇ H ₅ O ₂ S ⁻	thiosalicylic acid	ND	x	x						
157	C ₉ H ₁₇ O ₂ ⁻	pelargonic acid	ND	x				x	x		
167	C ₈ H ₇ O ₄ ⁻	dehydroacetic acid	ND								
169	C ₇ H ₅ OS ₂ ⁻	dithiosalicylic acid	ND	x							
171	C ₇ H ₇ O ₃ S ⁻ /C ₁₀ H ₁₉ O ₂ ⁻	toluenesulfonic acid/capric acid	ND	x	x						
183	C ₆ H ₃ N ₂ O ₃ S ⁻	diazobenzenesulfonic acid	ND	x							
185	C ₂ H ₂ IO ₂ ⁻ (?)	iodoacetic acid(?)	ND		x						

*Negative Mode Scan was not done for Vent 0 (ND = Not Determined)

M/Z	ASSIGNMENTS	COMMENTS	SITES				
			1	2	3	4	5
35	35Cl^-	possibly from chlorinated organic compounds	x	x	x	x	x
37	37Cl^-	possibly from chlorinated organic compounds	x	x	x	x	x
42	CNO^-	isocyanyl anion					
45	HCOO^-	formic acid	x	x			
55	$\text{C}_3\text{H}_3\text{O}^-$	acrolein					
57	CNS^-	thiocyanic acid				x	
59	$\text{C}_2\text{H}_5\text{O}_2^-$	acetic acid					
61	$\text{C}_2\text{H}_5\text{S}^-$	ethyl mercaptan					
69	$\text{C}_3\text{H}_2\text{O}_2^-$	propionic acid					
71	$\text{C}_3\text{H}_3\text{O}_2^-$	acrylic acid/Oxid. Prod. of mass 55					x
72	$\text{C}_2\text{H}_2\text{NS}^-$	methyl thiocyanate				x	x
73	$\text{C}_3\text{H}_5\text{O}^-$	propanoic acid					x
75	$\text{C}_2\text{H}_3\text{O}_5^-/\text{C}_2\text{H}_3\text{O}_3^-$	thio acetic acid/glycolic acid					
77	$\text{C}_2\text{H}_5\text{SO}^-$	ethyl sulfonic acid					
83	ClO_3^- (Cl=35)	chloric acid					x
85	ClO_3^- (Cl=37)/ $\text{C}_4\text{H}_5\text{O}_2^-$	chloric acid/crotonic acid or methacrylic acid				x	x
87	$\text{C}_3\text{H}_3\text{O}_3^-$	pyruvic acid					
89	$\text{C}_3\text{H}_6\text{O}_3^-$	lactic acid	x			x	x
91	$\text{C}_3\text{H}_7\text{SO}^-$	propyl mercaptan derivative	x	x	x	x	x
92	$(\text{C}_2\text{H}_5\text{NO}_3)^-$	ethyl nitrate anion					
93	$\text{C}_2\text{H}_5\text{SO}_2^-$	ethyl mercaptan derivative					
93	$\text{C}_6\text{H}_5\text{O}^-$	phenol					
95	$\text{CH}_3\text{O}_3\text{S}^-$	methanesulfonic acid					
99	$\text{C}_5\text{H}_7\text{O}_2^-$	carboxylic acid					
101	$\text{C}_5\text{H}_9\text{O}_2^-$	valeric acid or isovaleric acid				x	x
105	$\text{C}_4\text{H}_9\text{SO}^-$	butyl mercaptan derivative					
107	$\text{C}_3\text{H}_7\text{SO}_2^-$	propyl mercaptan					
107	$\text{C}_7\text{H}_9\text{O}^-$	cresol					
108	$\text{C}_6\text{H}_6\text{NO}^-$	nicotiny alcohol					
109	$\text{C}_2\text{H}_5\text{SO}_3^-$	ethyl mercaptans derivative					
111	$\text{C}_6\text{H}_7\text{O}_2^-$	sorbic acid					
115	$\text{C}_5\text{H}_7\text{O}_3^-/\text{C}_4\text{H}_3\text{O}_4^-/\text{C}_6\text{H}_{11}\text{O}_2^-$	levulinic acid/fumaric acid or maleic acid/n-caproic acid	x			x	x
121	$\text{C}_4\text{H}_9\text{SO}_2^-$	butyl mercaptan or ethyl sulfide					
121	$\text{C}_8\text{H}_9\text{O}^-/\text{C}_7\text{H}_5\text{O}_2^-$	benzoic acid/dimethylphenol					
122	$\text{C}_6\text{H}_4\text{NO}_2^-$	nitrosophenol or picolinic acid					
123	$\text{C}_3\text{H}_7\text{SO}_3^-$	propyl mercaptan derivative					
125	$\text{C}_2\text{H}_5\text{O}_4\text{S}^-$	ethyl sulfate or dimethyl sulfate					
127	$\text{C}_6\text{H}_4\text{ClO}^-/\text{C}_7\text{H}_{11}\text{O}_2^-$	chlorinated phenols/cyclohexane carboxylic acid				x	
129	$\text{C}_7\text{H}_{13}\text{O}_2^-$	heptanoic acid				x	
131	$\text{C}_7\text{H}_{15}\text{S}^-$	hepta mercaptan derivative					
135	$\text{C}_8\text{H}_7\text{O}_2^-$	toluic acid or phenylacetic acid					
135	$\text{C}_5\text{H}_{11}\text{SO}_2^-$	pentyl mercaptan derivative					
137	$\text{C}_4\text{H}_9\text{SO}_3^-$	butyl mercaptan, ethyl sulfide derivatives					
139	$\text{C}_7\text{H}_4\text{FO}_2^-(?)$	fluorobenzoic acid(?)					
141	$\text{C}_6\text{H}_5\text{O}_4^-(?)$	kojic acid(?)					
142	$\text{C}_6\text{H}_8\text{NOS}^-$	NI					
143	$\text{CH}_3(\text{CH}_2)_6\text{COO}^-$	caprylic acid				x	
153	$\text{C}_7\text{H}_5\text{O}_2\text{S}^-$	thiosalicylic acid					
157	$\text{C}_9\text{H}_{17}\text{O}_2^-$	pelargonic acid	x				
167	$\text{C}_8\text{H}_7\text{O}_4^-$	dehydroacetic acid					
169	$\text{C}_7\text{H}_5\text{O}_5\text{S}^-$	dithiosalicylic acid					
171	$\text{C}_7\text{H}_7\text{O}_3\text{S}^-/\text{C}_{10}\text{H}_{19}\text{O}_2^-$	toluenesulfonic acid/capric acid					
183	$\text{C}_6\text{H}_3\text{M}_2\text{O}_3\text{S}^-$	diazobenzenesulfonic acid					
185	$\text{C}_2\text{H}_2\text{IO}_2^-(?)$	iodoacetic acid(?)					

LEGEND

Site 1=	Tekawitha School
Site 2=	10 metres from gate
Site 3=	Line Ridge Road
Site 4=	StoneChurch Road and Upper Ottawa Street
Site 5=	Arbur Street

SUMMARY RESULTS OF CHEMICALS
TENTATIVELY IDENTIFIED WITHIN THE VENTS USING THE POSITIVE ION
MASS SPECTRAL ANALYSES

M/Z	ASSIGNMENTS	COMMENTS	VENTS									
			0	1	2	2A	2B	3	4	4A	4B	
29	C ₂ H ₅ ⁺	fragment										
30	H ₂ CO ⁺	methane derivative	x		x				x	x		
31	CH ₃ O ⁺	fragment		x		x						
32	(CH ₃ NH ₂)H ⁺	methylamine							x	x	x	
39	C ₃ H ₃ ⁺	fragment ion	x	x		x						
43	C ₂ H ₃ O ⁺	fragment ion				x				x	x	
44	C ₂ H ₅ NH ⁺	ethylenimine		x	x	x	x	x	x	x		
45	C ₂ H ₅ O ⁺	fragment	x									
46	[(CH ₃) ₂ NH]H ⁺	dimethylamine or ethylamine		x		x			x	x	x	
48	CH ₅ NO ⁺	methoxyamine		x		x						
49	CH ₅ S ⁺	methylmercaptan		x	x	x						
56	C ₃ H ₆ N ⁺	propionitrile		x		x					x	
57	C ₃ H ₅ O ⁺ /C ₄ H ₉ ⁺	acrolein or fragment		x	x			x			x	
58	(C ₃ H ₇ N)H ⁺	allylamine									x	
59	C ₃ H ₆ OH ⁺	acetone or fragment ion									x	
*60	(C ₃ H ₁₀ N) ⁺	acetamide and/or propanamine	x		x				x	x		
61	C ₃ H ₉ O ⁺ /C ₂ H ₅ O ₂ ⁺ /C ₂ H ₉ N ₂ ⁺	ethyl methylether, propyl alcohol/ methyl formate/ethylenediamine	x								x	
63	(C ₂ H ₆ O ₂)H ⁺	ethylene glycol					x				x	
65	(CH ₃ SH.OH) ⁺	methyl mercaptan derivative					x					
65	C ₅ H ₅ ⁺	fragment ion						x				
66	C ₅ H ₆ ⁺	fragment ion										
67	C ₅ H ₇ ⁺	cyclopentadiene									x	
69	C ₄ H ₅ O ⁺ /C ₃ H ₅ N ₂ ⁺	fragment or furan/pyrazole	x	x	x			x	x	x	x	
70	(C ₄ H ₇ N)H ⁺	butane nitrile				x						
71	(C ₄ H ₆ O)H ⁺	crotonaldehyde, methyl vinyl ketone				x	x					
72	C ₃ H ₆ NO ⁺	acrylamide or hydracrylonitrile		x	x			x				
74	(C ₄ H ₁₁ N)H ⁺ /(C ₃ H ₇ NO)H ⁺	butylamine/diethylamine/dimethylformamide				x						
75	[(CH ₃) ₂ N ₂ O]H ⁺ /[(C ₂ H ₅) ₂ O]H ⁺	dimethylnitrosoamine/diethylether or t-butanol		x		x	x				x	
*76	(C ₃ H ₉ NO)H ⁺	possibly an amino alcohol				x	x	x				
77	C ₃ H ₉ O ₂ ⁺	methyl cellosolve, or propylene glycol or trimethylene glycol				x						
79	(C ₂ H ₆ OS)H ⁺	dimethyl sulfoxide or 2-mercaptoethanol										
80	(C ₅ H ₅ N)H ⁺	pyridine		x	x	x	x		x	x	x	
81	C ₄ H ₅ N ₂ ⁺	pyrazine/pyridazine/pyrimidine		x	x							
82	C ₆ H ₁₀ ⁺	cyclohexane or 2,3-dimethyl-1,3-butadiene									x	
83	C ₅ H ₇ O ⁺ /C ₆ H ₁₁ ⁺	methylfuran or fragment or 2,3-dimethyl-1,3-butadiene	x	x	x	x	x	x	x	x		
85	C ₄ H ₅ O ₂ ⁺ /C ₅ H ₉ O ⁺	diketene/cyclopentanone	x	x	x	x	x	x	x	x	x	
87	(C ₄ H ₇ O ₂) ⁺ /C ₅ H ₁₁ O ⁺	methylacrylate or methacrylic acid/NI				x						
89	(C ₄ H ₈ O ₂)H ⁺ /(C ₅ H ₁₂ O)H ⁺	esters and/or alcohols		x				x				
*90	C ₄ H ₁₂ NO ⁺ /C ₃ H ₈ NO ₂ ⁺	2-amino-2-methyl-1-propanol/urethan				x	x					
93	(C ₃ H ₇ SH.OH) ⁺	propylmercaptan derivative				x						
93	C ₃ H ₉ O ₃ ⁺	glycerol										
*94	(C ₆ H ₇ N)H ⁺ /C ₆ H ₅ NH ₂)H ⁺	methyl pyridine/aniline		x			x	x			x	
95	(C ₂ H ₅ SHO ₂ H) ⁺ /[(CH ₃) ₂ SO ₂ H] ⁺	ethyl mercaptan and/or methyl sulfide derivatives		x	x	x						
95	(C ₅ H ₆ N ₂)H ⁺ /(C ₆ H ₆ O)H ⁺	aminopyridine/phenol						x	x	x		
96	C ₅ H ₆ NO ⁺	pyridine-1-oxide		x		x	x					
97	C ₅ H ₅ O ₂ ⁺ /C ₆ H ₉ O ⁺ /CH ₅ O ₃ S ⁺	furfural/l-pentol/methane sulfonic acid	x	x	x	x			x	x	x	
*99	C ₆ H ₁₁ O ⁺ /C ₅ H ₇ O ₂ ⁺ /C ₄ H ₃ O ⁺	cyclohexanone/lactone/maleic anhydride		x	x	x	x			x	x	
100	C ₆ H ₁₄ N ⁺	cyclohexylamine										
101	C ₆ H ₁₃ O ⁺ /C ₅ H ₉ O ₂ ⁺ /C ₄ H ₅ O ₃ ⁺	hexanone/ethylacrylate/succinic anhydride	x		x		x	x	x			
102	(C ₆ H ₁₅ N)H ⁺	alkylamine										
103	(C ₆ H ₁₄ O)H ⁺ /(C ₅ H ₁₀ O ₂)H ⁺	diisopropyl ether/propyl acetate/pyruvic acid, methyl ester/methyl butyrate		x				x			x	
104	C ₈ H ₈ ⁺	M ⁺ ion of styrene				x	x	x				
106	C ₄ H ₁₂ NO ₂ ⁺	2-amino-2-methyl-1,3-propanediol or diethanolamine	x									
107	(C ₇ H ₆ O)H ⁺	benzaldehyde			x		x		x	x		
*108	C ₇ H ₇ ⁺ .NH ₃ /C ₇ H ₁₀ N ⁺	tropylium-ammonia cluster/benzylamine or ethyl pyridine or methyl aniline	x	x	x	x	x				x	
109	C ₆ H ₅ O ₂ ⁺ /C ₇ H ₉ O ⁺	quinone/cresols		x	x							
110	C ₆ H ₈ NO ⁺	aminophenols	x		x	x	x				x	
111	C ₆ H ₇ NO ₂ ⁺	hydroquinone	x	x	x	x	x	x	x	x	x	
111	(C ₂ H ₅ SHO ₃ H) ⁺ , [(CH ₃) ₂ SO ₃ H] ⁺	ethylmercaptan or dimethylsulfide				x						
113	C ₄ H ₅ N ₂ O ₂ ⁺ /C ₆ H ₉ O ₂ ⁺ / C ₇ H ₁₃ O ⁺ /C ₆ H ₁₃ N ₂ ⁺	maleic hydrazide/sorbic acid/ cycloheptanone/triethylenediamine			x		x				x	

M/Z	ASSIGNMENTS	COMMENTS	0	1	2	2A	2B	3	4	4A	4B
115	(C ₇ H ₁₄ O) ⁺ H ⁺	2-heptanone									
116	(C ₅ H ₉ NS) ⁺ H ⁺ /C ₉ H ₈ ⁺	isobutyl thiocyanate/indene									
117	(C ₇ H ₁₆ O) ⁺ H ⁺ /(C ₆ H ₁₂ O ₂) ⁺	heptanol and/or butylacetate									
*118	C ₆ H ₁₆ NO ⁺	2-diethylaminoethanol									
119	C ₄ H ₇ O ₂ S ⁺ /C ₈ H ₇ O ⁺ / C ₆ H ₁₅ O ₂ ⁺	3-sulfolene/benzofuran									
*120	C ₅ H ₁₄ NO ₂ ⁺	cellosolve (2-butoxyethanol)									
121	C ₅ H ₁₃ O ₃ ⁺ /C ₈ H ₉ O ⁺	2-amino-2-ethyl-1,3-propanediol									
122	C ₈ H ₁₂ N ⁺	methyl carbitol/acetophenone									
123	C ₈ H ₁₁ O ⁺ /C ₇ H ₇ O ₂ ⁺	N.I.									
*124	C ₆ H ₆ NO ₂ ⁺	xlenol, phenethyl alcohol/benzoic acid									
125	C ₈ H ₁₃ O ⁺	nitrosophenol									
126	C ₈ H ₁₆ N ⁺ (?)	N.I.									
127	C ₃ H ₇ N ₆ ⁺ or C ₆ H ₇ O ₃ ⁺	coniceine (?)									
128	C ₅ H ₆ NO ₅ ⁺	melamine or pyrogallol									
129	C ₇ H ₁₃ O ₂ ⁺ /C ₈ H ₁₇ O ₂ ⁺	pyrithione									
130	C ₆ H ₁₂ NS ⁺	n-butyl acrylate/ethyl amyl ketone									
131	C ₇ H ₁₅ O ₂ ⁺ /C ₈ H ₁₉ O ⁺	or hexyl methyl ketone									
*132	C ₉ H ₁₀ N ⁺	isoamyl thiocyanate									
133	C ₉ H ₉ O ⁺ /C ₆ H ₁₃ O ₃ ⁺	ester/alcohol or ether									
*134		skatole									
135	C ₆ H ₁₅ SO ⁺	cinnamaldehyde, 2,2-dimethyl-1, 3-dioxolane-4-									
136	C ₇ H ₆ NS ⁺	methanol or 2,5-tetrahydrofuran(methanol)									
137	C ₈ H ₉ O ₂ ⁺ /C ₉ H ₁₃ O ⁺	hexylmercaptan or dipropyl sulfide derivatives									
138	C ₈ H ₁₂ NO ⁺	benzothiazole									
139	C ₈ H ₁₁ O ₂ ⁺ /C ₆ H ₇ N ₂ O ₂ ⁺ / C ₄ H ₁₁ O ₃ S ⁺	esters/alcohols, ethers									
140	C ₃ H ₁₀ NO ₃ S/C ₆ H ₆ NO ₃ ⁺	phenylethanamine									
141	C ₆ H ₁₃ N ₄ ⁺	cresols/nitroanilines/									
142	C ₈ H ₁₆ NO ⁺ (?)	2-(ethylsulfonyl) ethanol									
143	C ₈ H ₁₅ O ₂ ⁺	n-methyltaurine/nitrophenols									
144	C ₁₀ H ₁₀ N ⁺	methenamine (?)									
*145	C ₆ H ₉ O ₄ ⁺ /C ₈ H ₁₇ O ₂ ⁺ / C ₁₀ H ₉ O ⁺	n-acetylcyclohexylamine (?)									
*146	C ₉ H ₈ NO ⁺	cyclohexane carboxylic acid, methyl ester									
147	N.I.	naphthylamine									
*148	C ₈ H ₆ NO ₂ ⁺ (?)	fumaric acid, dimethyl ester or lactide/									
149	C ₈ H ₅ O ₃ ⁺	ester compound/naphthol									
150	C ₆ H ₁₆ NO ₃ ⁺	8-hydroxyquinoline									
151	C ₆ H ₁₅ O ₄ ⁺	N.I.									
152	C ₈ H ₁₀ NO ₂ ⁺	phthalimide (?)									
153	C ₈ H ₉ O ₃ ⁺	phthalic anhydride									
154	C ₇ H ₈ NO ₃ ⁺	triethanolamine									
155	C ₇ H ₇ O ₂ S ⁺ /C ₄ H ₁₃ FN ₂ O ₂ P ⁺ / C ₁₀ H ₁₉ O ⁺	triethylene glycol									
156	NI	acetaminophen									
157	C ₁₀ H ₂₁ O ⁺	cresotic acids									
158	C ₁₀ H ₂₄ N ⁺	amino salicylic acid									
159	C ₆ H ₇ O ₃ S ⁺	Thiosalicylic acid/Dimefox/-Terpineol/citronella									
160	C ₆ H ₁₀ NO ₂ S ⁺	NI									
161	NI	citronellol, menthol or rhodinol									
162	NI	Diisoamylamine									
163	C ₈ H ₁₉ SO ⁺	benzene sulfonic acid									
164	C ₆ H ₁₄ NO ₄ ⁺	cititolone									
165	C ₈ H ₉ N ₂ O ₂ ⁺ /C ₁₀ H ₁₃ O ₂ ⁺ / C ₁₁ H ₁₇ O ⁺	NI									
166	C ₁₀ H ₁₆ NO ⁺	octyl mercaptan or dibutylsulfide derivatives									
167	C ₉ H ₁₁ O ₃ ⁺ /C ₉ H ₁₅ N ₂ O ⁺	2-Nitro-2-propyl-1,3- propanediol									
168	C ₁₂ H ₁₀ N ⁺	phthalamide/ethylphenyl acetate/ Jasmone									
169	C ₈ H ₉ O ₄ ⁺	(aminopropyl) benzyl alcohol									
170	(C ₁₂ H ₁₁ N) ⁺	ethyl salicylate or ethyl vanillin/									
*171	C ₁₂ H ₁₁ O ⁺	5-amino-2-butoxypyridine									
172	C ₇ H ₁₁ ClN ₃ ⁺ /C ₈ H ₁₈ N ₃ O ⁺	carbazole									
173	C ₆ H ₉ N ₂ O ₂ S ⁺ /C ₁₀ H ₂₁ O ₂ ⁺	dehydroacetic acid									

M/Z	ASSIGNMENTS	COMMENTS	VENTS									
			0	1	2	2A	2B	3	4	4A	4B	
174	C ₆ H ₈ NO ₃ S ⁺	sulfanilic acid										
175	C ₇ H ₁₁ O ₅ ⁺	adipic acid, dimethyl ester or dimethoxane		x	x		x					
176	C ₆ H ₇ FO ₂ S ⁺	sulfanilyl fluoride					x					
177	C ₉ H ₂₁ SO ⁺	nonylmercaptan derivative		x			x			x	x	
178	C ₁₀ H ₁₂ NO ₂ ⁺	acetoacetanilide					x	x				
179	C ₈ H ₁₉ SO ₂ ⁺	octylmercaptan or dibutyl sulfide derivative					x	x				
180	C ₁₀ H ₁₄ NO ₂ ⁺	IPC						x				
181	C ₁₀ H ₁₃ O ₃ ⁺	2-phenoxyethanol acetate	x		x		x					
182	C ₁₂ H ₂₄ N ⁺	dicyclohexylamine			x	x	x					
183	C ₆ H ₁₇ FN ₂ OP ⁺										x	
	/C ₁₁ H ₁₉ O ₂ ⁺ /											
	C ₆ H ₁₅ O ₆ ⁺	mipafox/geraniol, formate/sorbitol										
184	C ₄ H ₁₁ NO ₃ PS ⁺	acephate	x	x							x	
185	C ₁₂ H ₁₃ N ₂ ⁺	benzidine		x							x	
186	C ₁₂ H ₂₈ N ⁺	tributylamine		x	x		x				x	
188	NI	NI										
190	C ₁₂ H ₁₆ NO ⁺ (?)	benzoylpiperidine, or ethyl crotonanilide(?)		x	x							
192	C ₁₂ H ₁₈ NO ⁺ /C ₁₃ H ₂₂ N ⁺	N,N-diethyl-m-toluidide/2,6-Di-tert butylpyridine			x		x					
193	C ₁₃ H ₂₁ O ⁺ /C ₁₂ H ₁₇ O ₂ ⁺	ionone/isoamyl benzoate			x		x					
194	C ₁₁ H ₁₆ NO ₂ ⁺	isobutyl-p-aminobenzoate				x	x			x		
196	C ₁₁ H ₁₇ NS ⁺	1-naphthol isothiocyanate		x	x		x					
197	C ₁₁ H ₁₄ ClO ⁺ /C ₁₂ H ₂₀ O ₂ ⁺	dowicide/geraniol, acetate or linalyl acetate			x				x			
	/											
198	C ₁₃ H ₁₂ NO ⁺	benzanilide	x									
199	(C ₁₂ H ₁₀ N ₂ O) ⁺ H ⁺	N-nitrosodiphenylamine	x									
201	C ₆ H ₅ N ₂ O ₆ ⁺	2,4-dinitroresorcinol		x							x	
202	C ₁₂ H ₁₂ NO ₂ ⁺	carbaryl		x							x	
203	C ₁₀ H ₁₉ O ₄ ⁺	ethyl adipate/hexyleneglycol, diacetate			x							
204	C ₉ H ₁₈ NO ₂ S ⁺ /C ₁₀ H ₂₂ NO ₅ ⁺	Lethane/pebulate		x	x		x				x	
206	NI	NI										
208	C ₁₂ H ₁₈ NO ₂ ⁺	promecarb			x					x		
214	C ₁₃ H ₁₂ NO ₂ ⁺	salicylanilide		x								
217	C ₁₁ H ₂₁ O ₄ ⁺	esters			x	x	x			x		
218	NI	NI										
219	C ₇ H ₇ O ₆ S ⁺	sulfosalicylic acid					x					
220	NI	NI					x					
221	C ₄ H ₈ Cl ₂ O ₄ P ⁺ /C ₁₁ H ₉ O ₅ ⁺			x			x					
	/C ₁₅ H ₂₅ O ⁺ SO ⁺	Dichlorvos/Purpurogallin/DBMC or santalol or butylated hydroxytoluene					x					
222	C ₁₂ H ₁₆ NO ₃ ⁺ /C ₁₃ H ₂₀ NO ₂ ⁺	carbofuran/bufencarb					x					
223	C ₁₀ H ₂₃ O ₃ S ⁺	decylmercaptan or dipentyl sulfide derivatives				x				x		
225	C ₁₀ H ₉ O ₄ S ⁺ /C ₇ H ₁₈ O ₆ P ⁺	cassella's acid or naphthol sulfonic acid/mevinphos/		x								
226	C ₁₃ H ₁₂ N ₃ O ⁺	Tinuvin P,		x								
234	NI	NI										
235	C ₁₃ H ₁₉ N ₂ O ₂ ⁺ /C ₁₇ H ₁₅ O ⁺									x		
	C ₈ H ₁₆ N ₂ O ₄ P ⁺ /C ₁₀ H ₁₇ N ₂ O ₅ S ₂ ⁺	lenacil/dibenzalacetone/ O,O-diethyl-O-(3-methyl-5-pyrazolyl)phosphate or Quinomethionate									x	
240	C ₁₀ H ₁₀ NO ₄ S ⁺ /C ₁₆ H ₁₇ NO ⁺	amino-naphthol-sulfonic acid/ diphenamid		x								
246	C ₁₃ H ₁₆ N ₃ O ₂ ⁺	pyrolan		x						x		
248	NI	NI		x						x		

SUMMARY RESULTS OF CHEMICALS TENTATIVELY IDENTIFIED WITHIN
THE RESIDENTIAL AREAS USING THE POSITIVE ION MASS SPECTRAL ANALYSES

M/Z	ASSIGNMENTS	COMMENTS	SITES				
			1	2	3	4	5
29	C ₂ H ₅ ⁺	fragment	x	x	x	x	x
30	H ₂ CO ⁺	methane derivative					x
31	CH ₃ O ⁺	fragment					x
32	(CH ₃ NH ₂)H ⁺	methylamine			x		
39	C ₃ H ₃ ⁺	fragment ion			x		
43	C ₂ H ₃ O ⁺	fragment ion	x	x	x	x	x
44	C ₂ H ₅ NH ⁺	ethylenimine					
45	C ₂ H ₅ O ⁺	fragment	x	x	x		x
46	[(CH ₃) ₂ NH]H ⁺	dimethylamine or ethylamine					
48	CH ₅ NO ⁺	methoxyamine					x
49	CH ₅ S ⁺	methylmercaptan					x
56	C ₃ H ₆ N ⁺	propanitrile					
57	C ₃ H ₅ O ⁺ /C ₄ H ₉ ⁺	acrolein or fragment			x	x	x
58	(C ₃ H ₇ N)H ⁺	allylamine					
59	C ₃ H ₆ OH ⁺	acetone or fragment ion		x	x	x	x
60	(C ₃ H ₁₀ N) ⁺	acetamide and/or propanamine					
61	C ₃ H ₉ O ⁺ /C ₂ H ₅ O ₂ ⁺ /C ₂ H ₉ N ₂ ⁺	ethyl methylether, propyl alcohol/ methyl formate/ethylenediamine		x	x		x
63	(C ₂ H ₆ O ₂)H ⁺	ethylene glycol					
65	(CH ₃ SH.OH) ⁺	methyl mercaptan derivative					
65	C ₅ H ₅ ⁺	fragment ion					
66	C ₅ H ₆ ⁺	fragment ion					
67	C ₅ H ₇ ⁺	cyclopentadiene			x		
69	C ₄ H ₅ O ⁺ /C ₃ H ₅ N ₂ ⁺	fragment or furan/pyrazole	x		x	x	x
70	(C ₄ H ₇ N)H ⁺	butane nitrile		x			
71	(C ₄ H ₆ O)H ⁺	crotonaldehyde, methyl vinyl ketone			x		x
72	C ₃ H ₆ NO ⁺	acrylamide or hydracrylonitrile			x	x	
74	(C ₄ H ₁₁ N)H ⁺ /(C ₃ H ₇ NO)H ⁺	butylamine/diethylamine/dimethylformamide					
75	[(CH ₃) ₂ N ₂ O]H ⁺ /[(C ₂ H ₅) ₂ O]H ⁺	dimethylnitrosoamine/diethylether or t-butanol			x		
76	(C ₃ H ₉ NO)H ⁺	possibly an amino alcohol					
77	C ₃ H ₉ O ₂ ⁺	methyl cellosolve, or propylene glycol or trimethylene glycol			x	x	x
79	(C ₂ H ₆ OS)H ⁺	dimethyl sulfoxide or 2-mercaptoethanol			x		
80	(C ₅ H ₅ N)H ⁺	pyridine					
81	C ₄ H ₅ N ₂ ⁺	pyrazine/pyridazine/pyrimidine			x		x
82	C ₆ H ₁₀ ⁺	cyclohexane or 2,3-dimethyl-1,3-butadiene					
83	C ₅ H ₇ O ⁺ /C ₆ H ₁₁ ⁺	methylfuran or fragment or 2,3-dimethyl-1,3-butadiene	x	x	x		x
85	C ₄ H ₅ O ₂ ⁺ /C ₅ H ₉ O ⁺	diketene/cyclopentanone	x	x	x		
87	(C ₄ H ₇ O ₂) ⁺ /C ₅ H ₁₁ O ⁺	methylacrylate or methacrylic acid/NI			x	x	x
89	(C ₄ H ₈ O ₂)H ⁺ /(C ₅ H ₁₂ O)H ⁺	esters and/or alcohols					
90	C ₄ H ₁₂ NO ⁺ /C ₃ H ₈ NO ₂ ⁺	2-amino-2-methyl-1-propanol/urethan				x	
93	(C ₃ H ₇ SH.OH) ⁺	propylmercaptan derivative					
93	C ₃ H ₉ O ₃ ⁺	glycerol					
94	(C ₆ H ₇ N)H ⁺ /C ₆ H ₅ NH ₂)H ⁺	methyl pyridine/aniline					
95	(C ₂ H ₅ SHO ₂ H) ⁺ /[(CH ₃) ₂ SO ₂ H] ⁺	ethyl mercaptan and/or methyl sulfide derivatives					
95	(C ₅ H ₆ N ₂)H ⁺ /(C ₆ H ₆ O)H ⁺	aminopyridine/phenol	x	x		x	x
96	C ₅ H ₆ NO ⁺	pyridine-1-oxide					
97	C ₅ H ₅ O ₂ ⁺ /C ₆ H ₉ O ⁺ /CH ₅ O ₃ S ⁺	furfural/1-pentol/methane sulfonic acid	x		x		x
99	C ₆ H ₁₁ O ⁺ /C ₅ H ₇ O ₂ ⁺ /C ₄ H ₃ O ⁺	cyclohexanone/lactone/maleic anhydride			x	x	x
100	C ₆ H ₁₄ N ⁺	cyclohexylamine					
101	C ₆ H ₁₃ O ⁺ /C ₅ H ₉ O ₂ ⁺ /C ₄ H ₅ O ₃ ⁺	hexanone/ethylacrylate/succinic anhydride					
102	(C ₆ H ₁₅ N)H ⁺	alkylamine					
103	(C ₆ H ₁₄ O)H ⁺ /(C ₅ H ₁₀ O ₂)H ⁺	diisopropyl ether/propyl acetate/pyruvic acid, methyl ester/methyl butyrate				x	x
104	C ₈ H ₈ ⁺	M ⁺ ion of styrene					
106	C ₄ H ₁₂ NO ₂ ⁺	2-amino-2-methyl-1,3-propanediol or diethanolamine					
107	(C ₇ H ₆ O)H ⁺	benzaldehyde					
108	C ₇ H ₇ ⁺ .NH ₃ /C ₇ H ₁₀ N ⁺	tropylum-ammonia cluster/benzylamine or ethyl pyridine or methyl aniline				x	
109	C ₆ H ₅ O ₂ ⁺ /C ₇ H ₉ O ⁺	quinone/cresols			x		x
110	C ₆ H ₈ NO ⁺	aminophenols					
111	C ₆ H ₇ NO ₂ ⁺	hydroquinone	x	x	x		x
111	(C ₂ H ₅ SHO ₃ H) ⁺ , [(CH ₃) ₂ SO ₃ H] ⁺	ethylmercaptan or dimethylsulfide					
113	C ₄ H ₅ N ₂ O ₂ ⁺ /C ₆ H ₉ O ₂ ⁺ / C ₇ H ₁₃ O ⁺ /C ₆ H ₁₃ N ₂ ⁺	maleic hydrazide/sorbic acid/ cycloheptanone/triethylenediamine					x

		1	2	3	4	5
115	(C ₇ H ₁₄ O)H ⁺					
116	(C ₉ H ₉ NS)H ⁺ /C ₉ H ₈ ⁺					
117	(C ₇ H ₁₆ O)H ⁺ /(C ₆ H ₁₂ O ₂)H ⁺					x
118	C ₆ H ₁₆ NO ⁺					
119	C ₄ H ₇ O ₂ S ⁺ /C ₈ H ₇ O ⁺ / C ₆ H ₁₅ O ₂ ⁺	x		x		x
120	C ₅ H ₁₄ NO ₂ ⁺			x		
121	C ₅ H ₁₃ O ₃ ⁺ /C ₈ H ₉ O ⁺					
122	C ₈ H ₁₂ N ⁺					
123	C ₈ H ₁₁ O ⁺ /C ₇ H ₇ O ₂ ⁺					
124	C ₆ H ₆ NO ₂ ⁺					x
125	C ₈ H ₁₃ O ⁺					
126	C ₈ H ₁₆ N ⁺ (?)					x
127	C ₃ H ₇ N ₆ ⁺ or C ₆ H ₇ O ₃ ⁺					
128	C ₅ H ₆ NO ₅ ⁺		x	x		x
129	C ₇ H ₁₃ O ₂ ⁺ /C ₈ H ₁₇ O ₂ ⁺					
130	C ₆ H ₁₂ NS ⁺					
131	C ₇ H ₁₅ O ₂ ⁺ /C ₈ H ₁₉ O ⁺					
132	C ₉ H ₁₀ N ⁺					x
133	C ₉ H ₉ O ⁺ /C ₆ H ₁₃ O ₃ ⁺					
134	N.I.					
135	C ₆ H ₁₅ SO ⁺					
136	C ₇ H ₆ NS ⁺					
137	C ₈ H ₉ O ₂ ⁺ /C ₉ H ₁₃ O ⁺					
138	C ₈ H ₁₂ NO ⁺					
139	C ₈ H ₁₁ O ₂ ⁺ /C ₆ H ₇ N ₂ O ₂ ⁺ / C ₄ H ₁₀ O ₃ S ⁺					
140	C ₃ H ₁₀ NO ₃ S/C ₆ H ₆ NO ₃ ⁺	x		x	x	x
141	C ₆ H ₁₃ N ₄ ⁺					
142	C ₈ H ₁₆ NO ⁺ (?)					
143	C ₈ H ₁₅ O ₂ ⁺					
144	C ₁₀ H ₁₀ N ⁺					
145	C ₆ H ₉ O ₄ ⁺ /C ₈ H ₁₇ O ₂ ⁺ / C ₁₀ H ₉ O ⁺					
146	C ₉ H ₈ NO ⁺			x		x
147	N.I.					
148	C ₈ H ₆ NO ₂ ⁺ (?)					
149	C ₈ H ₅ O ₃ ⁺					
150	C ₆ H ₁₆ NO ₃ ⁺		x	x		x
151	C ₆ H ₁₅ O ₄ ⁺					
152	C ₈ H ₁₀ NO ₂ ⁺					
153	C ₈ H ₉ O ₃ ⁺		x			
154	C ₇ H ₈ NO ₃ ⁺					
155	C ₇ H ₇ O ₂ S ⁺ /C ₄ H ₁₃ FN ₂ OP ⁺ / C ₁₀ H ₁₉ O ⁺					
156	NI					
157	C ₁₀ H ₂₁ O ⁺					
158	C ₁₀ H ₂₄ N ⁺			x		
159	C ₆ H ₇ O ₃ S ⁺	x		x		
160	C ₆ H ₁₀ NO ₂ S ⁺					
161	NI					
162	NI					
163	C ₈ H ₁₉ SO ⁺					
164	C ₆ H ₁₄ NO ₄ ⁺					
165	C ₈ H ₉ N ₂ O ₂ ⁺ /C ₁₀ H ₁₃ O ₂ ⁺ / C ₁₁ H ₁₇ O ⁺	x	x			
166	C ₁₀ H ₁₆ NO ⁺					
167	C ₉ H ₁₁ O ₃ ⁺ /C ₉ H ₁₅ N ₂ O ⁺					
168	C ₁₂ H ₁₀ N ⁺					
169	C ₈ H ₉ O ₄ ⁺					
170	(C ₁₂ H ₁₁ N)H ⁺				x	
171	C ₁₂ H ₁₁ O ⁺					
172	C ₇ H ₁₁ ClN ₃ ⁺ /C ₈ H ₁₈ N ₃ O ⁺					
173	C ₆ H ₉ N ₂ O ₂ S ⁺ /C ₁₀ H ₂₁ O ₂ ⁺					
	2-heptanone					
	isobutyl thiocyanate/indene					
	heptanol and/or butylacetate					
	2-diethylaminoethanol					
	3-sulfolene/benzofuran					
	cellosolve (2-butoxyethanol)					
	2-amino-2-ethyl-1,3-propanediol					
	methyl carbitol/acetophenone					
	N.I.					
	xylenol, phenethyl alcohol/benzoic acid					
	nitrosophenol					
	N.I.					
	conicefine (?)					
	melamine or pyrogallol					
	pyrithione					
	n-butyl acrylate/ethyl amyl ketone					
	or hexyl methyl ketone					
	isoamyl thiocyanate					
	ester/alcohol or ether					
	skatole					
	cinnamaldehyde, 2,2-dimethyl-1,3-dioxolane-4-methanol or 2,5-tetrahydrofuran-dimethanol					
	N.I.					
	hexylmercaptan or dipropyl sulfide derivatives					
	benzothiazole					
	esters/alcohols, ethers					
	phenylethanamine					
	cresols/nitroanilines/					
	2-(ethylsulfonyl) ethanol					
	n-methyltaurine/nitrophenols					
	methenamine (?)					
	n-acetylcyclohexylamine (?)					
	cyclohexane carboxylic acid, methyl ester					
	naphthylamine					
	fumaric acid, dimethyl ester or lactide/					
	ester compound/naphthol					
	8-hydroxyquinoline					
	N.I.					
	phthalimide (?)					
	phthalic anhydride					
	triethanolamine					
	triethylene glycol					
	acetaminophen					
	cresotic acids					
	amino salicylic acid					
	Thiosalicylic acid/Dimefox/-Terpineol/citronellal					
	NI					
	citronellol, menthol or rhodinol					
	Diisoamylamine					
	benzene sulfonic acid					
	citriolone					
	NI					
	NI					
	NI					
	octyl mercaptan or dibutylsulfide derivatives					
	2-Nitro-2-propyl-1,3-propanediol					
	phthalamide/ethylphenyl acetate/ Jasmone					
	(aminopropyl) benzyl alcohol					
	ethyl salicylate or ethyl vanillin/					
	5-amino-2-butoxypyridine					
	carbazole					
	dehydroacetic acid					
	diphenylamine					
	phenylphenol					
	crimidine/2-heptanone, semicarbazone					
	Porofof BSH/octyl acetate					

		1	2	3	4	5
174	C ₆ H ₈ NO ₃ S ⁺					
175	C ₇ H ₁₁ O ₅ ⁺					
176	C ₆ H ₇ FNO ₂ S ⁺					
177	C ₉ H ₂₁ SO ⁺					
178	C ₁₀ H ₁₂ NO ₂ ⁺					
179	C ₈ H ₁₉ SO ₂ ⁺					
180	C ₁₀ H ₁₄ NO ₂ ⁺					
181	C ₁₀ H ₁₃ O ₃ ⁺					
182	C ₁₂ H ₂₄ N ⁺					
183	C ₆ H ₁₇ FN ₂ OP ⁺ /C ₁₁ H ₁₉ O ₂ ⁺ / C ₆ H ₁₅ O ₆ ⁺					
184	C ₄ H ₁₁ NO ₃ PS ⁺					
185	C ₁₂ H ₁₃ N ₂ ⁺					
186	C ₁₂ H ₂₈ N ⁺					
188	NI					
190	C ₁₂ H ₁₆ NO ⁺ (?)					
192	C ₁₂ H ₁₈ NO ⁺ /C ₁₃ H ₂₂ N ⁺					
193	C ₁₃ H ₂₁ O ⁺ /C ₁₂ H ₁₇ O ₂ ⁺					
194	C ₁₁ H ₁₆ NO ₂ ⁺					
196	C ₁₁ H ₁₇ NS ⁺					
197	C ₁₁ H ₁₄ ClO ⁺ /C ₁₂ H ₂₀ O ₂ ⁺					
198	C ₁₃ H ₁₂ NO ⁺					
199	(C ₁₂ H ₁₀ N ₂ O) ⁺ H ⁺					
201	C ₆ H ₅ N ₂ O ₆ ⁺					
202	C ₁₂ H ₁₂ NO ₂ ⁺					
203	C ₁₀ H ₁₉ O ₄ ⁺					
204	C ₉ H ₁₈ NO ₂ S ⁺ /C ₁₀ H ₂₂ NO ₅ ⁺					
206	NI					
208	C ₁₂ H ₁₈ NO ₂ ⁺					
214	C ₁₃ H ₁₂ NO ₂ ⁺					
217	C ₁₁ H ₂₁ O ₄ ⁺					
218	NI					
219	C ₇ H ₇ O ₆ S ⁺					
220	NI					
221	C ₄ H ₈ Cl ₂ O ₄ P ⁺ /C ₁₁ H ₉ O ₅ ⁺ /C ₁₅ H ₂₅ O ⁺ SO ⁺					
222	C ₁₂ H ₁₆ NO ₃ ⁺ /C ₁₃ H ₂₀ NO ₂ ⁺					
223	C ₁₀ H ₂₃ O ₃ S ⁺					
225	C ₁₀ H ₉ O ₄ S ⁺ /C ₇ H ₁₈ O ₆ P ⁺					
226	C ₁₃ H ₁₂ N ₃ O ⁺					
234	NI					
235	C ₁₃ H ₁₉ N ₂ O ₂ ⁺ /C ₁₇ H ₁₅ O ⁺ C ₈ H ₁₆ N ₂ O ₄ P ⁺ /C ₁₀ H ₁₇ N ₂ O ₅ ⁺					
240	C ₁₀ H ₁₀ NO ₄ S ⁺ /C ₁₆ H ₁₇ NO ⁺					
246	C ₁₃ H ₁₆ N ₃ O ₂ ⁺					
248	NI					
	sulfanilic acid					
	adipic acid, dimethyl ester or dimethoxane					
	sulfanilyl fluoride					
	nonylmercaptan derivative					
	acetoacetanilide					
	octylmercaptan or dibutyl sulfide derivative					
	IPC					
	2-phenoxyethanol acetate					
	dicyclohexylamine			x		x
	mipafox/geraniol, formate/sorbitol					
	acephate					
	benzidine					
	tributylamine					
	NI					
	benzoylpiperidine, or ethyl crotonanilide(?)					
	N,N-diethyl-m-tolamide/2,6-Dl-tert					
	butylpyridine					
	ionone/isoamyl benzoate					
	isobutyl-p-aminobenzoate					
	1-naphthol isothiocyanate					
	dowicide/geraniol, acetate or linalyl				x	
	acetate					
	benzanilide					
	N-nitrosodiphenylamine					
	2,4-dinitroresorcinol					
	carbaryl					
	ethyl adipate/hexyleneglycol, diacetate					
	Lethane/pebulate					
	NI					
	promecarb					
	salicylanilide					
	esters				x	
	NI					
	sulfosalicylic acid					
	NI					
	Dichlorvos/Purpurogallin/DBMC or					
	santalol or butylated hydroxytoluene					
	carbofuran/bufencarb					
	decylmercaptan or dipentyl sulfide derivatives					
	cassella's acid or naphthol sulfonic acid/mevinphos/					
	Tinuvin P,					
	NI					
	lenacil/dibenzalacetone/					
	O,O-diethyl-O-(3-methyl-5-pyrazolyl)phosphate					
	or Quinomethionate					
	amino-naphthol-sulfonic acid/					
	diphenamid					
	pyrolan					
	NI					

5.0 CONCLUSIONS AND RECOMMENDATIONS

It is apparent that a large number of chemicals exist on the site. These chemicals are vented into ambient air at very small flow rates and volumes. From a chemical point of view, the richest vents are 2A and 2B which are thought to reach down to the old solidification pools. Vent #1 is a close runner-up in the complexity of the chemicals vented into ambient air. Based on these preliminary results, we conclude that:

- (a) A complex matrix of chemicals exists on the site.
- (b) Some of the chemicals are transported into the residential areas.
- (c) Based upon a preliminary and limited number of discrete samples, no PCBs or chlorinated pesticides were observed within the vents. This is confirmed by the TAGA™ results. Similarly no appreciable amounts of chlorinated benzenes were detected.
- (d) Due to the nature of some detected chemicals, we recommend that:
 - 1. Retrocalibration of a select number of chemicals be performed to estimate their concentration within an order of magnitude.
 - 2. Quantitative measurements be performed on site in order to determine the levels of "worst case" chemicals.

The large number of chemicals found on the site and transported into the residential areas precludes a complete retrocalibration and quantitative analysis. Hence, it was agreed that only twenty chemical species would be selected for further study. In order to select the most appropriate chemicals, it was agreed between SCIEX™ and the Landfill Study Group that a profiling of the detected chemicals be carried out. The resultant information is included in Appendix 2 under the headings of mass-to-charge (m/z), synonym, structure, uses, toxicity and Threshold Limit Value (TLV).

This information, especially the toxicity and TLV values will be used by the Study Group and SCIEX™ as a basis for the selection of twenty chemical species for further study as outlined in our recommendations.

APPENDIX I

Brief Report on Discrete Sample Analysis
by Wellington Environmental Consultants, Inc.



Wellington
Environmental
Consultants
Incorporated

291 Woodlawn Rd. W., Unit 2
P.O. Box 1261
Guelph, Ontario N1H 6N6
(519) 822-2436

January 6, 1982

Sciex Inc.,
55 Glencameron Rd.,
#202,
Thornhill, Ontario
L3T 1P2

ATTN: Dr. N. Hijazi

Dear Sir:

Enclosed please find a report describing the analyses carried out by our firm on the air samples collected at the Upper Ottawa St. landfill site.

Yours very truly,

B.G. Chittim

BGC/dec
Enclosure

AIR QUALITY MEASUREMENTS
UPPER OTTAWA ST. LANDFILL SITE

1. Introduction

Air samples were collected by Sciex personnel at the Upper Ottawa St. landfill site, Hamilton on August 21, 1981. The samples were subsequently analyzed by Wellington Environmental Consultants (WEC) and the following report summarizes the results.

2. Sampling

Air samples were collected from vents 1 and 2 at the landfill site using both passive badge monitors (charcoal; Dupont Pro-Tech^{RT}) and sorbent tubes (florisil and charcoal). The passive monitors were placed on the vent pipes and allowed to adsorb any compounds present. Samples taken using the sorbent tubes involved drawing a measured volume of air through the sorbent material in the tubes.

3. Analysis

The sorbent material in the badges and tubes was then removed and the adsorbed contaminants desorbed with solvent. These extracts were then analyzed for PCBs, chlorinated pesticides (12 selected) and chlorinated benzenes using capillary gas-liquid chromatography with an electron capture detector (GLC/ECD).

4. Results

- i) No PCBs (<10ng total) were detected in any of the sorbents. Assuming a volume of 100 of air was sampled, our limits of detection for PCBs using this method is $0.1 \mu\text{g}/\text{m}^3$. In comparison the NIOSH/OSHA standard for PCBs is $0.5 \text{ mg}/\text{m}^3$ (TWA).

- ii) The air extracts were analyzed for 12 common chlorinated pesticides (including Mirex). Of these, only one, Lindane, was detected and its level was very close to our limits of detection (ie. $<0.1 \mu\text{g}/\text{m}^3$).
- iii) As with the chlorinated pesticides only trace levels of a few chlorinated benzenes (1,3,5-trichlorobenzene in particular) were detected in the air extracts. Again, the levels found were virtually our detection limits ($0.1 \mu\text{g}/\text{m}^3$).

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APPENDIX 2

Profile of Detected Chemicals, Uses, Toxicity and TLV's

Chemicals Detected in the Positive Ion Mode - 2A

Chemicals Detected in the Negative Ion Mode - 2B

Appendices 2A and 2B provide six distinct types of information:

- (1) The masses (m/z) and the tentatively identified compounds associated with these masses; (positive and negative ions).
- (2) Alternate names and structure or molecular formulae of the compounds whenever available.
- (3) Data on uses and man made sources.
- (4) Data on toxicological effects of exposing these compounds to human beings whenever available.
- (5) Threshold Limit Values (T.L.V.) whenever available for the protection of human exposure.


The above information have been carefully extracted from the published literature. The length of data for each compound is by no means a measure of the relative importance of a compound, but more likely a reflection of the amount of available material published on the specific compound.

The chemical list is arranged in ascending mass to charge values, (M/Z), and are believed to be present in the Hamilton Landfill site.

REFERENCES SITED




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POSITIVE MODE





<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
30	methane	marsh gas/methyl hydride	CH_4	constituent of illuminating and cooking gas; in the manufacture of hydrogen, hydrogen cyanide, ammonia, acetylene, formaldehyde (3)	simple asphyxiant (3)	suggested: 10,000 ppm (5)
32	methylamine	methanamine	CH_3NH_2	in tanning and in organic syntheses (3)	irritating to eyes, skin & respiratory tract (3)	10 ppm (1)
44	ethylenimine	azacyclopropane		in the manufacture of triethylenemelamine (3)	FDA has declared this substance a carcinogen. Strongly irritating to eyes, skin & mucous membranes. Can be a skin sensitizer. (3)	0.5 ppm (1)
46	dimethylamine	N-methyl methanamine	$(\text{CH}_3)_2\text{NH}$	as accelerator in vulcanizing rubber, tanning, manuf. detergent soaps, or attracting boll weevils to exterminate them (3)	irritating to skin and mucous membranes	10 ppm (1)
46	ethylamine	ethanamine	$\text{C}_2\text{H}_5\text{NH}_2$	In resin chemistry; stabilizer for rubber latex; intermediate for dyestuffs, medicinals; in organic syntheses. (3)	Irritating to skin, mucous membranes, respiratory tract. (3)	10 ppm (1)
48	methoxyamine	O-methylhydroxylamine	CH_3ONH_2	analytical reagent for aldehydes and ketones. (3)	strong irritant (3)	Data not available.
49	methylmercaptan	methanethiol	CH_3SH	Data not available	narcosis, cyanosis, convulsions, pulmonary irritation; respiratory paralysis; headaches, nausea. (2)	10 ppm/ 15 mg/m ³ (2)

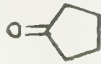
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56	propionitrile	propane nitrile	$\text{CH}_3\text{CH}_2\text{CN}$	Data not available	May cause dizziness, rapid respiration, headache, drowsiness, drop in blood pressure & pulse, and unconsciousness, delayed symptoms, chronic exposure may result in eye irritation, loss of appetite, mental deterioration (2)	6 ppm (NIOSH value) (6).
57	acrolein	2-propenal	$\text{CH}_2=\text{CHCHO}$	manufacture colloidal forms of metals; making plastics, perfumes (3). Also used as an aquatic herbicide (7).	Irritates skin, eyes and mucous membranes. Vapors cause lacrimation. A weak sensitizer; inhalation may cause asthmatic reaction. Inhalation of high conc'ns causes pulmonary edema.	0.1 ppm (1)
58	allylamine	2-propen-1-amine	$\text{CH}_2=\text{CHCH}_2\text{NH}_2$	in the manufacture of mercurial diuretics. (3)	a strong irritant to eyes, Data not available (6) mucous membranes, can cause excitement, convulsions, death. (3)	
59	acetone	2 propanone	CH_3COCH_3	Solvent for fats, oils, waxes, resins, rubber, plastics, lacquers, varnishes, rubber cements. (3)	prolonged or repeated topical use may cause erythema, dryness. Inhalation may produce headache, fatigue, excitement. (3)	1000 ppm (2)
60	acetamide	acetic acid amide	CH_3CONH_2	Solvent; solubilizer, plasticizer, stabilizer. Manufacture of methylamine, denaturing alcohol. In organic syntheses. (3)	No skin/eye irritation (6), Carcinogenic (6) Drowsiness, fatigue, nausea, acidosis, skin eruptions may occur upon exposure to cpd. (6)	Not available (6)
60	propanamine	-		no data available	no data available	none available

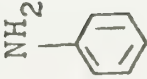
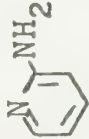


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61	ethylmethylether	methoxyethane	$C_2H_5OCH_3$	Data not available	No data available	No data available.
61	propyl alcohol	1-propanol	$CH_3(CH_2)OH$	Solvent for resins and cellulose esters. (3)	Mildly irritating to eyes, mucous membranes; depressant action similar to ethyl alcohol (3)	200 ppm (1)
61	methyl formate			Fumigant and larvicide for tobacco, dried fruits, cereals, etc. (3)	inhalation of vapor produces nasal and conjunctival irritation, retching, narcosis, death from pulmonary irritation. (3)	100 ppm (1)
61	ethylenediamine	1,2-ethanediamine	$H_2N(CH_2)_2NH_2$	Solvent for casein, albumin, shellac, and sulfur; emulsifier; stabilizing rubber latex; as inhibitor in antifreeze solutions (3)	because of its caustic nature and irritating properties, can cause nasal irritation, sensitization dermatitis, irritation of the respiratory system. (3)	10 ppm (1)
63	ethylene glycol	1,2-ethanediol	$HOCH_2CH_2OH$	Antifreeze in cooling and heating systems. Solvent in paints, and plastics industries. Softening agent for cellophane. (3)	Constitutes a hazard when ingested, e.g. drinking of antifreeze fluid. Transient stimulation of CNS followed by depression; vomiting, drowsiness, coma, respiratory failure. May proceed to death. (3)	lethal dose: 1.4ml/kg or 100 ml (3)
65	methyl mercaptan derivative		CH_5SO^+	-	-	-

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67	cyclopentadiene	1,3-cyclopentadiene		manuf resins; in organic syntheses, synthetic alkaloids, camphors. (3)	irritating to the eyes and nose. (3)	75ppm (1)
69	furan	divinylene oxide or furfuran		no data available	vapors are narcotic, can be absorbed through skin (3)	not pertinent
69	pyrazole	1,2-diazole		no data available	no data available	no data available
70	butane nitrile	propyl cyanide or butyronitrile		no data available	highly toxic (3)	P.O.L: 50 ppm (3)
71	crotonaldehyde	trans 2-butenal		in organic syntheses, as solvent in purification of mineral oils, manuf of resins, rubber antioxidants, insecticides (3)	highly irritating to eyes, skin and mucous membranes (3)	2ppm (6)
71	methyl vinyl ketone	3-buten-2-one	$\text{CH}_3\text{COCH}=\text{CH}_2$	commercial starting material for plastics (3)	readily absorbed through skin causing general poisoning of the organism. Irrit to mucous membranes and respiratory tract (3)	data not available (6)
72	hydracrylo-nitrile	3-hydroxy-propanenitrile		solvent for some cellulose esters and many inorganic salts (3)	no data available	no data available
72	acrylamide	propenamide	$\text{CH}_2=\text{CHCONH}_2$	no data available	highly toxic and irritant. Causes CNS paralysis. Can be absorbed through unbroken skin (3)	0.3 mg/m3 (4)

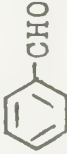

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74	butylamine	1-amino-butane	$\text{CH}_3(\text{CH}_2)_3\text{NH}_2$	intermediate for pharmaceuticals, dyestuffs rubber chemicals, emulsifying agents, insecticides, synthetic tanning agents (3)	potent skin, eye, mucous membrane irritant. Direct skin contact causes severe primary irritation and blistering (3)	5ppm (1)
74	diethylamine	n-ethylethanamine	$(\text{C}_2\text{H}_5)_2\text{NH}$	in the rubber and petroleum industry; in resins, dyes pharmaceuticals (3)	may be irritating to skin, mucous membranes (3)	25ppm (1)
74	dimethylformamide	DMF	$(\text{CH}_3)_2\text{N}-\overset{\text{O}}{\parallel}\text{C}$	solvent for liqs and gases. In the synthesis of organic compounds, solvent for orlon and similar polyacrylic fibers. (3)	vapour harmful. Irritant to eyes, skin and mucous membranes. Liver injury has been produced in experimental animals by prolonged inhalation of 100ppm (3)	100ppm (1)
75	dimethylnitrosoamine			no data available	no data available	
75	diethylether			no data available	no data available	
75	t-butanol	3-butanol		not data available	no data available	
77	propylene glycol	1,2-propandiol	$\text{CH}_3\underset{\text{OH}}{\underset{ }{\text{CH}}}\text{CH}_2\text{OH}$	as non-toxic antifreeze in breweries and dairy establishments. In the manuf of synthetic resins as mist to disinfect air (3)	Therap cat: pharmaceutical aid (humectant solvent). Liquid may irritate eyes (3)	not pertinent (6)
77	methylcellulose®	2-methoxyethanol	$\text{HO}(\text{CH}_2)_2\text{OCH}_3$	solvent for low-viscosity cellulose acetate, natural and synthetic resins, and some alcohol-soluble dyes; sealing moisture-proof cellophane, nail polishes, wood stains (3)	may cause anemia, macrocytosis, appearance of young granulocytes in blood; also CNS symptoms. Readily absorbed through skin (3)	25ppm (1)


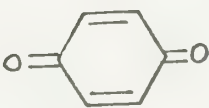
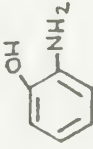

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77	trimethylene-glycol	1,3-propanediol	$\text{HO}(\text{CH}_2)_3\text{OH}$	no data available	exposure may cause coldness, spastic contraction of muscles, loss of reflexes, coma, death, pulmonary edema, eye irritation. Chronic exposure may cause weakened reflexes. (3)	none available (6)
79	dimethyl sulfide	methylsulfoxide or DMSO	CH_3SOCH_3	solvent for acetylene, sulfur dioxide and gases. As paint and varnish remover (3)	slight eye irritation may occur (6)	not available (6)
79	2 mercaptoethanol	nothioglycol		no data available	no data available	
80	pyridine			as a solvent for anhydrous mineral salts, in organic syntheses, and in analytical chemistry (3)	may cause CNS depression, irritation of skin and respiration tract. Large dose may produce GI disturbances, kidney and liver damage (3)	5ppm (1)
81	pyrazine	1,4-diazine		no data available	no data available	
81	pyridazine	1,2-diazine		no data available	no data available	
81	pyrimidine	1,3-diazine		no data available	no data available	
82	cyclohexane	hexahydrobenzene		solvent for lacquers and resins. Paint and varnish remover. In fungicidal formulations (3)	high concns may act as narcotic, skin irritant (3)	300ppm (1)
82	2,3-dimethyl-1,3-butadiene	diisopropenyl	$\text{CH}_2=\text{C}(\text{CH}_3)-\text{CH}=\text{CH}_2$	in manuf of synthetic rubber and polymers (3)	no data available	
83	methyl furan		$\text{C}_4\text{H}_3\text{OCH}_3$	no data available	no data available	not pertinent

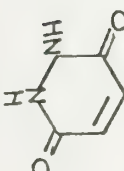
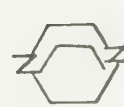

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85	diketene		$(CH_2=C=O)_2$	monomer is used for the conversion of higher acids into their anhydrides; for acetylation in the manuf of cellulose acetate and aspirin (3)	monomer is a severe pulmonary irritant causing pulmonary edema if inhaled (3)	none available
85	cyclopentanone	ketocyclopentane		no data available	no data available	
87	methylacrylate	2-propenoic acid methyl ester	$CH_2=CH-C(=O)-OCH_3$	monomer in manuf of leather finish resins, textile and paper coatings, and plastic films (3)	the monomer is highly irritating to eyes, skin, mucous membranes. Lethargy and convulsions may occur if vapors of monomer are inhaled in high concns. (3)	10ppm(1)
87	methacrylic acid	2-methyl propenoic acid	$CH_2=C(CH_3)-COOH$	manuf of methacrylate resins and plastics (3)	may act as a strong irritant (3)	not pertinent (5)
90	2-amino-2-methyl-1-propanol		$\begin{array}{c} NH_2 \\ \\ CH_3-C-CH_2OH \\ \\ CH_3 \end{array}$	in synthesis of surface active agents, vulcanization accelerators, pharmaceuticals as emulsifying agent for cosmetic creams and lotions, mineral oil, polishes, cleaning compounds (3)		
90	urethan	carbamic acid ethyl ester	$\begin{array}{c} O \\ \\ NH_2-C-OC_2H_5 \end{array}$	molten urethan is a good solvent for various organic materials. As solubilizer and cosolvent for pesticides, fumigants (3)	Therap Cat: antineoplastic (3)	
93	glycerol	1,2,3-propanetriol		as solvent, humectant, plasticizer, sweetener. In manuf of cosmetics, liquors, confectioneries, lubricants, as antifreeze, in shock absorber fluids (3)	Therap Cat: Pharmaceutical aid (humectant; solvent) (3)	

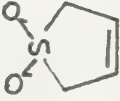
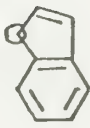
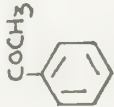
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94	methylpyridine	picoline		no data available	severe skin & eye irritation, narcosis, headache, nausea, giddiness, vomiting. Chronic exposure may result in occasional vomiting and diarrhea, weight loss and anemia (3)	not available
94	aniline	benzenamine		manuf dyes, medicinals, resins, varnishes, perfumes, shoe blacks, vulcanizing rubber, as solvent	intoxication may occur from inhalation, ingestion, or cutaneous absorption. Acute: cyanosis, methemoglobinemia, vertigo, headache, mental confusion (3)	0.5ppm (1)
95	aminopyridine			manuf. of drugs and dyes (3)	inhalation may cause headaches, dizziness, nausea. Flush extremities and high blood pressure may result from skin adsorption (2)	0.5ppm (2)
96	pyridine-1-oxide			synthetic intermediate (3)	no data available	
97	furfural	2-furancarboxaldehyde		in the manuf of furfuralphenol plastics such as durite; in solvent refining of petroleum oils. In the manuf of varnishes; as insecticides, fungicide, germicide (3)	irritates mucous membranes and acts on CNS. Causes lacrimation, inflammation of eyes, irritation of throat, headache (3)	5ppm (2)

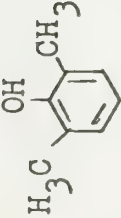

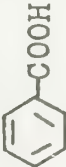

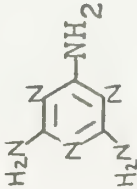
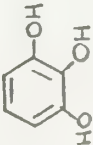
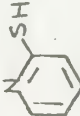
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97	1-pentol	3-methyl-2-penten-4-yn-1-ol	<chem>HC#CC(=C)CH2OH</chem> <chem>CC(C)C=CCO</chem>	intermediate in Vitamin A synthesis (3)	both isomers tend to polymerize and will explode when heated above 120° in a sealed bomb tube (3)	none available
97	methanesulfonic acid	methylsulfonic acid	<chem>CH3SO2OH</chem>	as a catalyst in polymerization, alkylation and esterification as a solvent (3)	strong irritant (3)	
99	cyclohexanone		<chem>O=C1CCCCC1</chem>	solvent for cellulose acetate, nitrocellulose, natural resins, crude rubber, waxes, fats, DOT. In prod of adipic acid for nylon (3)	irritating to eyes, mucous membranes (3)	50ppm (1)
99	lactone			no data available	no data available	
99	maleic anhydride	2,5-furandione	<chem>O=C1C=CC(=O)O1</chem>	in organic syntheses, manuf of alkyl-type of resins, dye intermediates, agricultural chemicals, pharmaceuticals (3)	powerful irritant, causes burns. Inhalation can cause pulmonary edema. Avoid contact with skin, eyes (3)	0.25ppm (1)
100	cyclohexylamine	aminocyclohexane	<chem>Nc1ccccc1</chem>	in organic synthesis, manuf insecticides, plasticizers, rubber chemicals, dyestuffs, dry-cleaning soaps (3)	can cause irritation and sensitization. High concn's cause nausea and narcotic effects (3)	10ppm, 1972 (5)
101	hexanone	methylisobutyl ketone		no data available	200 ppm; eye irritation 400; nasal irritation inhalation: survived: 2,000 ppm, 4hr death: 400 ppm, 4hr (2)	100 ppm (2)
101	succinic anhydride	dihydro-2,5-furandione	<chem>O=C1OC(=O)CC1=O</chem>	no data available	no data available	
101	ethyl acrylate	2-propenoic acid ethyl ester		in manuf. of water emulsion paint vehicles, textile and paper coatings leather finish resins and adhesives (3)	monomer is highly irritating to eyes, skin, mucous membranes. Lethargy and convulsions may occur if vapors of monomer are inhaled in high concn's. (3)	25 ppm (1)

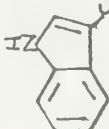
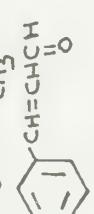
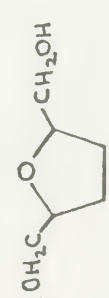
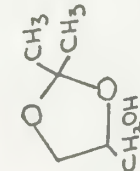

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103	diisopropyl ether			no data available	no data available	
103	methyl butyrate	butanoic acid methyl ester		manuf. artificial rum and fruit essences (3)	no data available	
103	propyl acetate			manuf. flavors, perfumes. Solvents for resins, cellulose derivatives and plastics. (3)	may be irritating to skin, mucous membranes, and in high concn's narcotic (3)	200 ppm (1)
104	styrene	ethenyl benzene		manuf. plastics; synthetic rubber; resins; insulator (3)	may be irritating to eyes mucous membranes, and in high concns, narcotic (3)	100 ppm (1)
106	2-amino-2-methyl-1,3-propanediol		$ \begin{array}{c} \text{NH}_2 \\ \\ \text{HOCH}_2\text{CCH}_2\text{OH} \\ \\ \text{CH}_3 \end{array} $	in synthesis of surface active agents. As emulsifying agent for cosmetic creams and lotions, mineral oil and paraffin wax, polishes, cleaning compounds (3)	no data available	
106	diethanolamine	2,2'-Iminobis ethanol	$ (\text{HOCH}_2\text{CH}_2)_2\text{NH} $	as rubber chemicals intermediate, in surface active agents used in textile specialities, herbicides, petr demulsifiers. In various agricultural chemicals, cosmetics (3)	Vapors may cause moderate irritation, skin contact may cause first-degree burns on short exposure and may cause secondary burns on long exposure (6)	not pertinent
107	benzaldehyde	benzenecarbonal		manuf. of dyes, perfumery, cinnamic and mandelic acids; as solvent; in flavors (3)	narcotic in high concn's May cause contact dermatitis. (3)	not available (6)
108	benzylamine	α -aminotoluene		in organic syntheses (3)	highly irritating to skin, mucous membranes (3)	


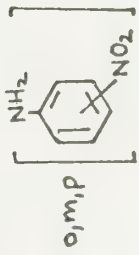
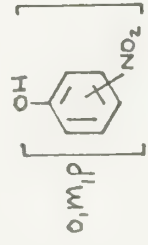
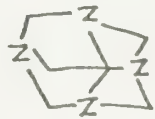
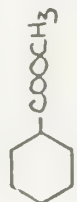
<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
108	ethyl pyridine			no data available	no data available	
108	methyl aniline	N-methylbenzenamine		biodegradation: decomposition by a soil microflora (3)	severe toxic effects: 40 ppm, 60 min. Symptoms of illness, 10 ppm. Unsatisfactory, 5 ppm	5 ppm 1974 (5)
109	quinone	2,5-cyclohexadiene-1,4-dione		oxidizing agent; in photography; manuf. dyes; tanning hides; strengthening animal fibers (3)	can cause dermatitis, erythema, formation of papules and vesicles. Vapors acting on eye can cause conjunctivitis and corneal ulceration (3)	0.1 ppm (1)
109	cresols			as disinfectant like phenol; also as a solvent (3)	inhalation can cause depression, resp. failure; dyspnea (3)	5ppm (2)
110	aminophenols	hydroxy aniline		manuf of azo and sulfur dyes; dyeing furs and hairs (3)	no data available	
111	hydroquinone			as photographic reducer and developer (3)	dermatitis can result from skin contact. Staining and opacification of cornea occur in workers exposed for prolonged periods to concn's of vapor not high enough for prod of systemic effects (3)	2mg/m ³ (2)

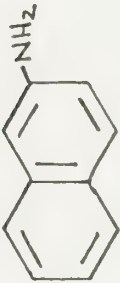

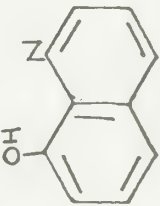
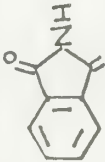
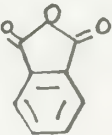
<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
113	maleic hydrazide	1,2-dihydro-3,6-pyridazinedione		as photographic reducer and developer (3)	Inhalation of dust causes irritation of nose & throat. Contact with skin or eyes causes irritation (3)	Not available (6)
113	sorbic acid	2,4-hexadienoic acid		mold and yeast inhibitor. Fungistatic agent for foods, especially cheeses. To improve characteristics of drying oils. (3)	no data available	
113	cycloheptanone	ketoheptamethylene		no data available	no data available	
113	triethylenediamine	1,4-diazabicyclo (2.2.2)octane		catalyst in making urethane foams (3)	no data available	
115	2-heptanone	methylamyl ketone	$\text{CH}_3(\text{CH}_2)_4\text{COCH}_3$	in perfumery as constituent of artificial camation oils; as industrial solvent (3)	no data available	100 ppm, 1974 (5)
116	isobutyl thiocyanate	isobutyl sul focyante		no data available	no data available	
116	indene	indonapthene		found in tars from coal, lignite and crude petroleum. Used in paint and coating mfg. chemical synthesis intermediate (3)	Slight skin & eye irritation. Irritation of mucuous membranes & lungs, pulmonary edema. Chronic exposure may cause dermatitis, liver & kidney damage (6)	10 ppm, 45mg/m ³ (6)
117	heptanol	n-heptyl alcohol		no data available	low toxicity, liquid may irritate eyes (6)	not available (6)
117	butylacetate	acetic acid 1,1-dimethylethyl ester	$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2$	as gasoline additive (3)	mild eye and nose irritation : 200-300 ppm. unsatisfactory >200 ppm symptoms of illness: 500ppm severe toxic effects: 2,000 ppm, 60 min. (5)	200 ppm (1)


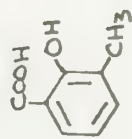

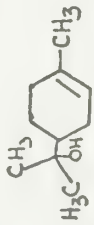
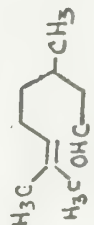
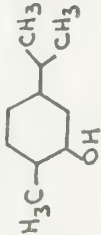
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118	2-diethyl amino ethanol	2,hydroxy triethylamine	$(C_2H_5)_2NCH_2CH_2OH$	no data available	severe skin & eye irritation, Dermatitis, weight loss, slight increase in clotting time. (3)	10 ppm (6)
119	3-sulfolene	2,5-dihydrothiophene 1,1-dioxide		organic solvent (3)	no data available	
119	benzofuran	coumarone		manuf. of coumarone-indene resins (3)	no data available	
119	butyl cellosolve®	2-butoxyethanol		solvent for nitrocellulose resins, grease, oil, albumin; dry cleaning (3)	Inhalation can result in kidney damage; brain damage eye irritation. (3)	50 ppm (1)
120	2-amino-2ethyl 1,3propanediol		$\begin{array}{c} NH_2 \\ \\ CH_2OHCH_2OH \\ \\ CH_2CH_3 \end{array}$	in synthesis of surface active agents, pharmaceutical. As emulsifying agent for cosmetic creams and lotions, mineral oil, paraffin wax, polishes, dry cleaning compounds (3)	no data available	
121	methyl carbitol®	2-(2-methoxyethoxy) ethanol		solvent for nitrocellulose, lacquers and dopes; in varnish removers, cleaning solutions, dye baths. (3)	no data available	
121	acetophenone	1-phenyl ethanone		in perfumery, catalyst for polymerization of olefins, in organic synthesis, esp. as a photosensitizer. (3)	Therap Cat: Hypnotic (3) Nototoxicity expected from inhalation or ingestion except slight narcotic effect. Liquid can cause eye & skin irritation on contact. (6)	Not available (6)

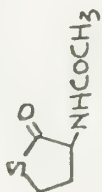

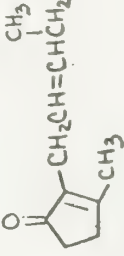
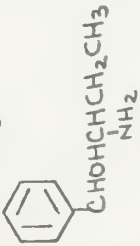
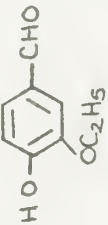
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123	xylenol	dimethylphenol		for the prep. of coal tar disinfectants; manuf. of artificial resins (3)	Vapor irritates eyes, nose & throat, and is readily absorbed through mucous membranes & lungs, producing general toxic symptoms (weakness, dizziness, headache, difficult breathing, twitching) (6)	45 ppm (6)
123	phenethyl alcohol	2-phenyl ethanol		in flavors and perfumery (3)	Therap Cat: Pharmaceutical aid (antimicrobial agent) (3)	
123	benzoic acid	benzene carboxylic acid		preserving foods, fats, fruit juices, alkaloidal sol'ns. in dyes; for curing tobacco (3)	Mild irritant to skin, eyes and mucous membranes (6)	Not pertinent (6)
124	nitrosophenol			no data available	can cause skin irritation, sensitization. (3)	
126	coniceine			no data available	no data available	
127	melamine	1,3,5-triazine-2,4,6-triamine		forms synthetic resins with formaldehyde (3)	no data available	
127	pyrogallol	1,2,3 benzene triol		developer in photography, as mordant for wool, staining leather, process engraving; manuf. various dyes, furs, hairs (3)	Ingestion may cause severe G.I. irritation, renal and hepatic damage, hemolysis convulsions, circulatory collapse, death (3)	
128	pyrithione	1-hydroxy-2(1H)-pyridinethione		fungicide, bactericide (3)	Therap Cat: Zinc deriv. as antibacterial; topical antifungal; anti seborrheic (3)	

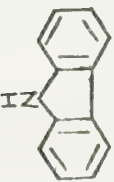
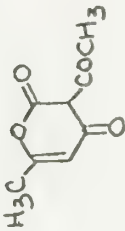
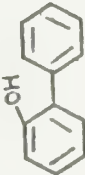
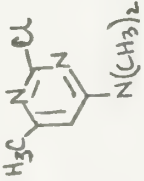
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129	n-butyl acrylate	2-propenoic acid butyl ester	$\text{CH}_2=\text{CH}-\text{C}(=\text{O})-\text{OC}_4\text{H}_9$	the monomer in the manuf. of polymers and resins for textile and leather finishes, paint formulations. (3)	Vapor is irritating when breathed at high concentrations. Contact with liquid causes irritation of skin & burning of eyes (6)	Data Not available (6)
129	ethyl amyl ketone	5-methyl-3-heptanone		solvent for nitrocellulose-alkyd nitrocellulose-maleic, and vinyl resins. (3)	narcotic in high concentrations (3)	25 ppm (1)
129	hexyl methyl ketone	2-octanone	$\text{CH}_3(\text{CH}_2)_5\text{C}(=\text{O})\text{CH}_3$	no data available	no data available	not pertinent
130	isoamylthiocyanate	isoamyl sul focyante	$(\text{CH}_3)_2\text{CH}(\text{CH}_2)_2\text{SCN}$	no data available	no data available	
132	skatole	3-methyl-1H-indole		constituent of beetroot nectandra, wood and coal tar (3)	no data available	
133	cinnamaldehyde	3-phenyl-2-propenal		in flavor and perfume industry (3)	no data available	
133	2,5-tetrahydrofuran-dimethanol	THF glycol		solvent, softener, humectant. In the synthesis of plasticizers, resins, surfactants, agricultural chemicals (3)	highly irritating to eyes skin, mucous membranes (3)	
133	2,2-dimethyl-1,3-dioxolane-4-methanol			versatile solvent and plasticizer (3)	no data available	
135	hexylmercaptan derivative		$\text{C}_6\text{H}_{15}\text{SO}^+$	no data available	no data available	
135	dipropyl sulfide		$\text{C}_3\text{H}_7-\text{S}-\text{S}-\text{C}_3\text{H}_7$	no data available	no data available	
136	benzothiazole			photographic dye mfg; rubber chemicals mfg. (3)	no data available	

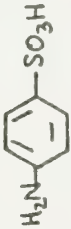
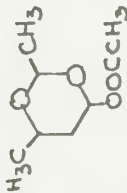
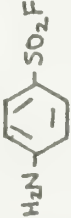
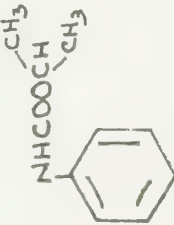
<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
138	phenylethanolamine		$\text{HOCH}_2\text{CH}_2\text{NH}_2$ 	free base as a stopping agent during polymerization of styrene-butadiene rubber; in hardening of waxes. Intermediate in the manuf. of pressor amines. (3)	no data available	
139	nitroanilines			dyestuff intermediate (3)	Highly toxic; absorbed through skin. Avoid breathing dust. Acute exposure can cause methoglobinemia, cyanosis (5)	1 ppm, 1974 (5)
139	2-ethyl sulfonyl ethanol			intermediate for pharmaceuticals, plasticizers, solvents. Humectant. Antistatic agent for synthetic fibers and fabrics (3)	no data available	
140	methyltaurine	2-methylamino ethane sulfonic acid	$\text{CH}_3\text{NH}(\text{CH}_2)_2\text{SO}_3\text{H}$	intermediate in the manuf. of surface active agents (3)	no data available	
140	nitrophenols			manuf. of many important compounds; as indicator in 2% alcohol solutions (3)	Moderate eye & mucous membrane irritation, C.N.S. depressant. Inhalation or ingestion causes headache, drowsiness, nausea & cyanosis. Can be absorbed through skin to give same symptoms as for inhalation. (6)	None available
141	methenamine	1,3,5,7-tetrazatricyclo [3.3.1.1 ^{3,7}]-decane		in adhesives, coatings, and sealing compounds; as dye fixative; as stabilizer for lubricating and insulating oils (3)	Therap Cat: antibacterial (urinary) (3)	
142	n-acetyl cyclohexylamine			no data available	no data available	
143	cyclohexane carboxylic acid, methyl ester			solubilizer for vulcanized rubber, clarifier for mineral oil; in insecticide formulations. (3)	no data available	

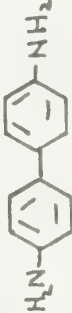
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144	naphthylamine			manuf. dyes (3)	harmful dust and vapor. The FDA has declared this substance a carcinogen. (3)	Not available (6)
145	fumaric acid, dimethyl ester	(E)-butenedioic acid	$\begin{array}{c} \text{HOOCCH} \\ \\ \text{HCCOOH} \end{array}$	substitute for tartaric acids in beverages and baking powders. As an antioxidant. Manuf. polyhydric alcohols, synthetic resins. As mordant in dyeing. (3)	no data available	unsatisfactory >.01 mg/m ³ (5)
145	naphthol	hydroxy naphthalene		manuf. dyes, perfumes, intermediates, the largest use is probably in making antioxidants for the synthetic rubber industry. (3)	Local action may produce peeling of the skin which may be followed by persistent pigmentation. Ingestion of large quantities may cause nephritis, lens opacity, vomiting and diarrhea abdominal pain, circulatory collapse, death. (3)	None available (6)
146	8-hydroxyquinoline	8-quinolinol		as fungistat, also as a chelating agent (3)	Carcinogen stimulation of CNS, digestive system irritation, eye irritation (6)	None available (6)
148	phthalimide	1 H-Isoindole-1,3 (2H)-dione		no data available	no data available	
149	phthalic anhydride	1,3-isobenzofurandione		manuf. phthalateins, phthalates, benzoic acid, synthetic indigo, artificial resins (glyptal) (3)	Vapor is moderately irritating, skin contact may cause first degree burns on short exposure, and secondary burns on long exposure (6)	2 ppm (1)

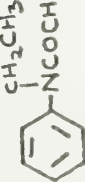
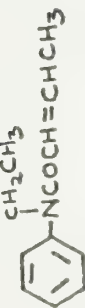
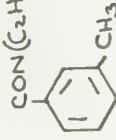
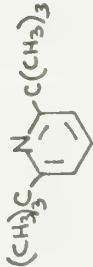
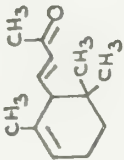
<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
150	triethanolamine	trihydroxytriethylamine	$(\text{HOCH}_2\text{CH}_2)_3\text{N}$	intermediate in manuf. of surface active agents, textile specialties, waxes, polishes, herbicides, petroleum demulsifiers, toilet goods. Solvent for shellac, dyes; manuf. synthetic resins. (3)	liquid may irritate eyes and skin (6)	Not pertinent (6)
151	triethylene glycol	triglycol	$\text{CH}_2\text{OCH}_2\text{CH}_2\text{OH}$ $\text{CH}_2\text{OCH}_2\text{CH}_2\text{OH}$	in various plastics to increase pliability; in air disinfection (3)	very low acute and chronic toxicity (5)	Not pertinent (6)
152	acetaminophen	4'-hydroxy acetanilide		manuf. azo dyes, photographic chemicals (3)	Therap Cat: analgesic antipyretic (3)	
153	cresotic acid			in manuf. of dyes (3)	Toxicity similar to salicylic acid. (i.e. absorption of large amounts can cause vomiting, abdominal pain, inc. resp., acidosis. May also cause skin rashes. (3)	
155	thiosalicylic acid	2-mercapto benzoic acid		manuf. thioindigo dyes (3)	no data available	
155	Dimefox	tetramethyl phosphorodiamidic fluoride	$(\text{CH}_3)_2\text{N}-\text{P}(=\text{O})-\text{N}(\text{CH}_3)_2$	pesticide (3)	a highly toxic cholinesterase inhibitor, symptoms similar to parathion, q.v. (3)	Oral LD50= 1-2mg/kg (8)
155	terpineol	α , α , 4-trimethyl-3-cyclohexene-1-methanol		perfumes; denaturing fats for soap manufacture (3)	Therap Cat: antiseptic (3)	
155	citronellal	3,7-dimethyl-6-octenal		in soap perfumes; insect repellent (3)	no data available	
157	menthol	5-methyl-2- (1-methylethyl) cyclohexanol		in liquors, confectionery, perfumery, cigarettes, cough drops, and nasal inhalers (3)	Therap Cat: topical antipruritic (3)	
157	citronellol	3,7,-dimethyl-6-octene 1-ol		in perfumery (3)	no data available	

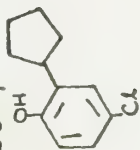
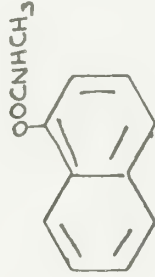
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
157	rhodinol			in perfumery (3)	no data available	
158	diisoamylamine	3-methyl-N- (3-methyl butyl)-1 butanamine		no data available	irritating to skin, mucous membranes. Has pressor effect (3)	
159	benzene sulfonic acid			manuf. phenol by fusion with NaOH. (3)	Highly irritant to skin, eyes, mucous membranes (3)	
160	citriolone	2-acetamido-4-mercaptobutyric acid γ -thiolactone		photographic antifogging agent (3)	no data available	
163	octyl mercaptan derivative		$C_8H_{19}SO^+$	no data available	no data available	
164	2-nitro-2-propyl-1,3-propanediol			as fat-reduction additive in feed (3)	no data available	
165	phthalamide	1,2-benzene dicarboxamide		no data available	no data available	
165	ethyl phenyl acetate	benzeneacetic acid ethyl ester		in perfumery (3)	no data available	
165	jasmone	3-methyl-2-(2-pentenyl)-2-cyclopenten-1-one		in perfumery (3)	no data available	
166	(aminopropyl) benzylalcohol			no data available	no data available	
167	ethyl salicylate	salicylic acid ethyl ester		manuf. artificial perfumes (3)	no data available	
167	ethyl vanillin	3-ethoxy-4-hydroxybenzaldehyde		in flavoring and perfumery (3)	no data available	

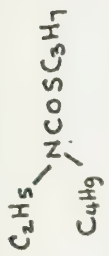
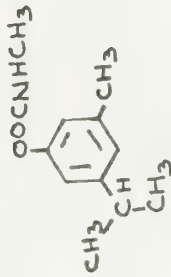
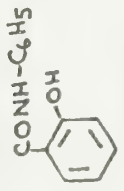
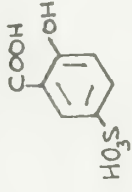
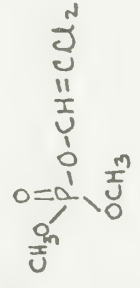
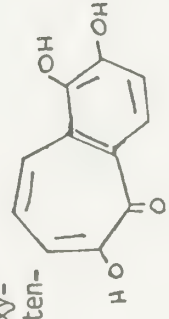
<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
167	5-amino-2-butoxy pyridine			no data available	no data available	
168	carbazole	9-azafluorene		important dye intermediate. Used in making photographic plates sensitive to ultraviolet light (3)	no data available	
169	dehydroacetic acid			in organic syntheses; as plasticizer, compatible with nitro-, cellulose, polystyrene methacrylate, vinylite resins; as fungicide and bacteriacide; in antienzyme toothpastes (3)	causes impaired kidney function. Large doses can cause vomiting, ataxia, convulsions (3)	
170	diphenylamine	N-phenylbenzene amine		manuf. dyes; stabilizing nitro-cellulose explosives and celluloid. In anal. chem for the detection of NO ₃ , ClO ₃ and other oxidizing substances (3)	may be irritating to mucous membranes. Overexposure, including ingestion of solid or skin contact, may cause fast pulse, hypertension and bladder trouble. Contact with dust irritates eyes (6)	10 mg/m ³ (6)
171	phenyl phenol	O-hydroxybiphenyl		as intermediate in the manufacture of resins; also in the rubber industry (3)	no data available	
172	crimidine	2-chloro-N,N,6-trimethyl-4-pyrimidinamine		rodenticide (3)	may cause serious CNS damage leading to fatal convulsions (3)	
172	2-heptanone semicarbazone			in perfumery as constituent of artificial camation oils; as industrial solvent (3)	no data available	

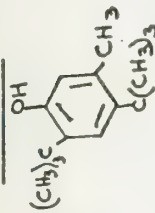
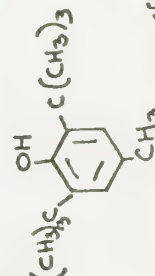
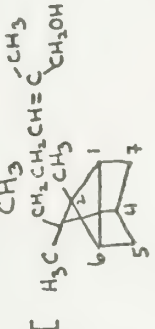
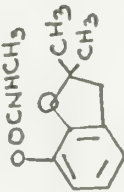
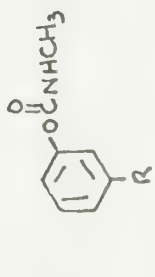
M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
173	Porofor® BSH	benzene sulfonic acid hydrazide		gas generating agent for use in making foam rubber and foam plastics. (3)	no data available	
173	octyl acetate	acetic acid α -ethyl hexyl ester		solvent for nitrocellulose, some resins, waxes and oils (3)	no data available	
174	sulfanilic acid	4-aminobenzene sulfonic acid		manufacture various dyes and organic chemicals (3)	Therap Cat: antibacterial (3)	
175	adipic acid, dimethyl ester			manufacture artificial resins, plastics (nylon), urethan foams. Used in baking powders instead of tartaric acid, cream of tartar. As an intermediate in lubricating oil additives. (3)	no data available	
175	dimethoxane	2,6-dimethyl-1,3-dioxan-4-ol acetate		preservative for cutting oils, resins, emulsions, water-based paints, cosmetics, inks. Gasoline additive. (3)	no data available	
176	sulfanilyl fluoride	p-aminobenzene sulfonyl fluoride		in the prep'n of dyes which pick up light readily (3)	no data available	
177	nonyl mercaptan derivative		$C_9H_{21}SO^+$	no data available	no data available	
178	acetoacetanilide	3-oxo-N-phenylbutanamide		manufacture of yellow dyes, such as Hansa and benzidine yellows. In rubber compounding. In organic syntheses. (3)	no data available	
179	octyl mercaptan derivative		$CH_3(CH_2)_7SH$	no data available	no data available	
180	ICP	phenyl carbamic acid 1-methyl ethyl ester		weed killer, applied as a spray to the soil (3)	no data available	

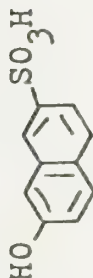
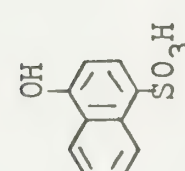
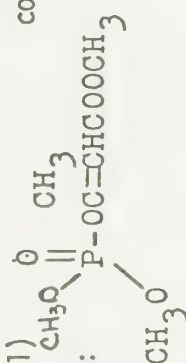
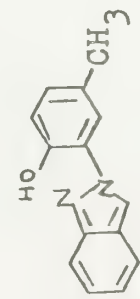
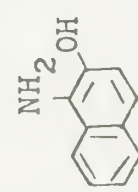
<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
181	2-phenoxyethanol acetate			fixative for perfumes in org. synthesis; as bacteriacide in conjunction with quaternary ammonium cpds; as insect repellant (3)	no data available	
182	dicyclohexylamine	N-cyclohexyl cyclohexanamine		in organic synthesis, manufacture. insecticides, plasticizers, corrosion inhibitors, rubber chemicals, dyestuffs, emulsifying agents, dry-cleaning soaps, acid gas absorbents (3)	a skin irritant and possible sensitizer (3)	20 ppm (suggested) (6)
183	Mipafox	N,N'-Bis(1-methylethyl) phosphorodiamidic fluoride	$ \begin{array}{c} \text{(CH}_3\text{)}_2\text{CHNH} \text{---} \text{P(=O)} \text{---} \text{CHNH} \\ \text{F} \qquad \qquad \qquad \text{(CH}_3\text{)}_2\text{CHNH} \end{array} $	insecticide (3)	cholinesterase inhibitor	
183	geraniol formate			as constituent of artificial neroli oil and of artificial orange blossom oil. (3)	no data available	
183	sorbitol	D-glucitol	$\text{CH}_2\text{OH}(\text{HCOH})_4\text{CH}_2\text{OH}$	in manufacture of sorbose, ascorbic acid, propylene glycol, synthetic plasticizers and resins; as moisture conditioner on printing rolls, in leather, tobacco. In writing inks. In antifreeze mixtures with glycerol or glycols. (3)	Therap Cat: Pharmaceutic aid (sweetening agent; tablet excipient). (3) Hot liquid will burn skin. (6)	Not pertinent (6)
184	acephate	acetylphosphoramidodithioic acid O,S-dimethyl ester	$ \begin{array}{c} \text{O} \qquad \qquad \text{O} \\ \parallel \qquad \parallel \\ \text{CH}_3\text{C} \text{---} \text{NH} \text{---} \text{P} \text{---} \text{OCH}_3 \\ \qquad \qquad \qquad \qquad \qquad \qquad \text{SCH}_3 \end{array} $	contact and systemic insecticide (3)	No teratogenic effects noted in rats and rabbits, except for slight moderate effects on cholinesterase depression (7)	
185	benzidine	4,4'-diamino biphenyl		manufacture dyes; as a reagent for H_2O_2 in milk and for detection of blood. (3)	FDA has declared this substance and its salts as carcinogens. (3)	


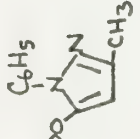
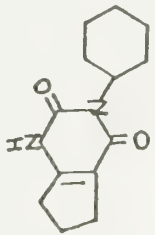
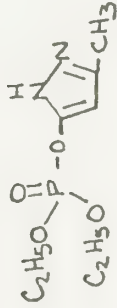
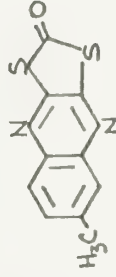
<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
186	tributylamine	N,N-dibutyl-1-butanamine	$[\text{CH}_3(\text{CH}_2)_3]_3\text{N}$	no data available	causes CNS stimulation, skin irritation, sensitization. (3)	P.O.L. 10 ppm
190	benzoylpiperidine			no data available	no data available	
190	ethylcrotonanilide			no data available	Therap Cat: antipruritic (3)	
192	N,N-diethyl-m-tolamide	N,N-diethyl-3-methylbenzamide		insect repellent (3)	Irritant to eyes, mucous membranes, but not to skin. Ingestion can cause CNS disturbances. (3)	
192	2,6-di-tert-butylpyridine			has been proposed as an additive for lubricating oil, gasoline and for stabilizing Cl-containing polymers. (3)	no data available	
193	ionone	α-cyclocitrylidene acetone		in perfumery (3)	may cause allergic reactions (3)	
193	isoamylbenzoate			in perfumery and cosmetics (3)	no data available	
194	isobutyl-p-aminobenzoate			no data available	no data available	

<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
196	1-naphthyl isothiocyanate	1-isothiocyanato naphthalene	$C_{10}H_7N=C=S$	has been used with pyrethrum as insecticide (3)	hepatotoxic; may cause dermatitis (3)	
197	dowicide	4-chloro-2-cyclopentyl phenol		germicide (3)	no data available	
197	geraniol acetate			no data available	no data available	
197	linalyl acetate	3,7-dimethyl-1,6-octadien-3-yl acetate		in perfumery (3)	no data available	
198	benzanilide	N-phenylbenzamide		manufacture dyes and perfumes (3)	no data available	
199	nitrosodiphenyl amine			accelerator in vulcanizing rubber (3)	no data available	
201	2,4 dinitro resorcinol	2,4-dinitro-1,3-benzene diol		for dyeing fabrics mordanted with iron. As a reagent for Co and for Fe (3)	no data available	
202	carbaryl	1-naphthalenol methyl carbamate		contact insecticide (3)	Data not available (6)	5mg/m ³ (6) oral LD50 = 400-850 mg/kg (8)
203	ethyl adipate	hexanedioic acid diethyl ester		no data available	no data available	
203	hexylene glycol diacetate	2-methyl-2,4-pentanediol		in cosmetics, hydraulic brake fluids (as coupling agent to castor oil) (3)	no data available	
204	lethane	thiocyanic acid 2-(2-butoxyethoxy) ethyl ester		insecticide (3)	moderately irritating to skin and mucous membranes, 91 mg/kg and, in high concn's narcotic. (3)	Oral LD50 = 91 mg/kg (8)

M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
204	pebulate	butyl ethyl thio carbamic acid S- propyl ester		selective herbicide (3)	rapidly metabolised in rats; about 50% of the radio-labelled cpd. administered was expired as CO ₂ in 3 days; about 25% in urine and 5% in faeces, (7)	Oral LD50 = 921-1120 mg/kg (8)
208	promecarb	3-methyl-5-(1-methyl ethyl) phenol methyl carbamate		insecticide (3)	cholinesterase inhibitor (3)	
214	salicylanilide			anti-mildew, fungicide (3)	In conc'd form, may cause irritation of skin, mucous membranes. (3)	
219	sulfosalicylic acid	3-carboxy-4-hydroxybenzene sulfonic acid		as metal chelating agents intermediate in the manufacture of surface active agents, organic catalysts and grease additives (3)	Irritating to skin, mucous membranes. (3)	
221	dichlorvos	phosphoric acid 2,2-dichloro ethenyl dimethyl ester		insecticide (3)	Inhalation may cause nuosis, ache eyes, rhinorrhea. Skin/eye contact may cause, nausea, diarrhea, sweating paralysis, low BP, convulsions. (2)	1mg/m ³ (1)
221	purpurogallin	2,3,4,6-tetrahydroxy-5H-benzocyclohepten-5-one		as an additive to edible or inedible fats or oils, hydrocarbon fuels or lubricants, retards oxidation or metal contamination (3)	no data available	

M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
221	D8VC	2,4-bis (1,1-dimethyl ethyl)-5-methyl phenol		intermediate in the production of rubber chemicals modified phenolic resins (3)	no data available	
221	butylated hydroxy toluene	2,6-bis (1,1- dimethyl- ethyl)-4- methyl phenol		antioxidant for food, animal feed petrol products, synthetic rubbers, plastics, animal and vegetable oils, soaps. Antiskinning agent in paints and inks. (3)	no data available	
221	santalol	5-(2,3-dimethyltricyclo[2.2.1.0] hept-3-yl)-2-methyl-2-penten-1-ol		In perfumes, soaps and detergents (3).no data available		
222	carbofuran			systemic insecticide, acaricide, nematocide (3)	anti cholinesterase (Reversible). Low to highly toxic. Ing. Inh. or dermal absorption may cause constriction of pupils, salivation, profuse sweating, nausea, vomiting, diarrhea (8)	Oral LD50= 8-14 mg/kg (8)
222	bufencarb	3-(1-ethylpropyl) phenol methyl carbamate mixture with 3-(1-methyl butyl) phenyl methyl carbamate mixture with 3-(1-methyl butyl) phenyl methyl carbamate (1:3)		soil and foliage insecticide (3)	Toxic if ingested or absorbed through skin, it inhibits cholinesterase activity in red blood cells (7)	
223	decyl mercaptan derivative		$C_{10}H_{22}SO_3^+$	no data available	no data available	
223	dipentyl sulfide			no data available	no data available	

<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
225	cassella's acid	7-hydroxy-2-napthalene sulfonic acid		dyestuff intermediate (3)	no data available	
225	napthol sulfonic acid			preparation of azo dyes (3)	no data available	
225	mevinphos	3-[(dimethoxy phosphinyloxy)-2-butenic acid methyl ester. Trade name: Phosdrin		contact and systemic insecticide (3)	cholinesterase inhibitor (3)	
226	tinuvin®p.	2-(2H-benzotriazol-2-yl)-4-methyl-phenol		an ultraviolet light absorber for stabilizing plastics and other organic materials against discoloration and deterioration. Effective in protecting polyesters, acrylates, dyes, synthetic and natural fibers, waxes, detergent sol'n, cosmetic formulations (3)	no data available	
240	amino-napthol-sulfonic acid			manuf. of azo dyes (3)	Irritating to eyes, skin, mucous membranes. (3)	


<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
240	diphenamid	N,N-dimethyl α -phenyl benzene acetamide		herbicide (3)	No contact effect to existing plants. Harmful if swallowed (7)	
246	pyrolan	dimethylcarbamic acid 3-methyl-1-phenol-1H- pyrazol-5-yl ester		insecticide (3)	cholinesterase inhibitor	
235	lenacil	3-cyclohexy-6,7-dihydro -1-H cyclopentapyrimidine- 2,4-(3H,5H)-dione		herbicide (3)	no data available	
235	dibenzalacetone	1,5-diphenyl-1,4-pentadien -3-one		in sun protection preparation (3)	no data available	
235	0,0-diethyl-0- (3-methyl-5- pyrazolyl) phosphorothioate			insecticide (3)	cholinesterase inhibitor (3)	
235	quinomethionate	6-methyl-1,3-dithiols [4,5-b]-quinoxalin-2- one		acaricide, fungicide (3)	no data available	

T.L.V. = Threshold Limit Values
P.O.L. = Provisional Operational Limit

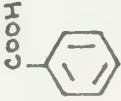
Catalog of chemicals with generic and chemical names and structures, uses and toxicity information.

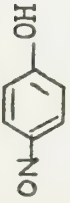
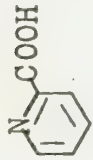
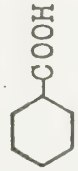

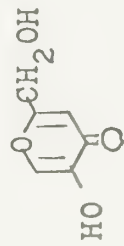
<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
45	fomic acid		$\begin{array}{c} \text{O} \\ \\ \text{HC}-\text{OH} \end{array}$	decalcifier, reducer in dyeing wool fast colours, dehairing and plumping hides, tanning, in sizes, electroplating, coagulating rubber latex, also in chemical analysis (3)	dangerously caustic to skin! Chronic absorption has been reported to cause albuminuria, hematuria (3)	5ppm (1)
55	acrolein	2-propenal	$\text{CH}_2=\text{CH}-\text{CHO}$	manuf colloidal forms of metals; making plastics, perfumes; warming agent in methyl chloride refrigerator. Used in organic syntheses. (3) Also used as an aquatic herbicide (7)	irritates skin, mucous membranes. Vapors cause lacrimation. A weak sensitizer; inhalation may cause asthmatic reaction. Inh. of high concns causes pulmonary edema. (3)	0.1ppm (1)
57	thiocyanic acid			no data available	no data available	
59	acetic acid	ethanoic acid		food processing plants; organic chemical mfg; nylon, fiber, dye-stuff and pigments mfg; rubber mfg., photographic chemicals & plastics mfg. (3)	Ing may cause severe corrosion of mouth and GI tract, with vomiting, diarrhea, circulatory collapse, eye irritation (3)	10ppm (1)
61	ethylmercaptan		$\text{C}_2\text{H}_5\text{SH}$	no data available	inhalation causes headache, nausea, muscle irritation, skin or eye contact result in paralysis, pulmonary irritation, liver/kidney damage (2)	10ppm (2)
69	propionic acid	2-propynoic acid		no data available	no data available	
71	acrylic acid	2-propenoic acid		in the manuf. of plastics (3)	strong irritant (3)	P.O.L.= 20ppm (5)
72	methyl thiocyanate	methyl sulfo cyanate	$\text{CH}_3\text{SC}\equiv\text{N}$	no data available	moderate skin, eye & mucous membrane irritation. Thiocyanate intoxication (6)	none available (6)

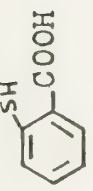
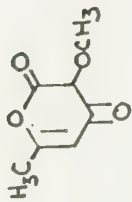
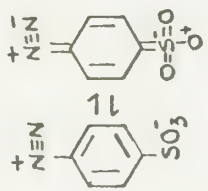
<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
73	propanoic acid	propionic acid or methylacetic acid	$\text{CH}_3\text{CH}_2\text{COOH}$	no data available	liquid causes skin & eye burns. Vapors may irritate eyes, nose & throat, but should not cause systemic illness (6)	toxicity by inhalation: 10ppm (6)
75	thioacetic acid	ethanethioic acid	CH_3CSH	no data available	no data available	
75	glycolic acid	hydroxy acetic acid	$\text{HOCH}_2\text{C}(=\text{O})\text{OH}$	in the processing of textiles, leather and metals; in pH control; in manuf. of adhesives, decontamination cleaning, dyeing (3)	mild irritant to skin and mucous membranes (3)	
77	ethyl sulfonic acid			no data available	no data available	
83	chloric acid		ClHO_3	oxidizing agent; with H_2SO_3 as catalyst in acrylonitrile polymerization (3)	strongly irritating to skin and mucous membranes (3)	not available
85	crotonic acid	2-butenic acid		manuf. of co-polymers with vinyl acetate used in lacquers and paper sizing; in the manuf. of softening agents for synthetic rubber (3)	no data available	
85	methacrylic acid	2-methylpropenoic acid	$\text{CH}_2=\text{C}(\text{CH}_3)\text{COOH}$	manuf of methacrylate resins and plastics (3)	may act as a strong irritant. (3)	not pertinent (5)
87	pyruvic acid	2-oxopropanoic acid	$\text{CH}_3\text{C}(=\text{O})\text{COOH}$	intermediate in sugar metabolism and in enzymatic carbohydrate degradation where it is converted to acetaldehyde and CO_2 by carbocylase (3)	no data available	
89	lactic acid	2-hydroxy propanoic acid	$\text{HO}-\text{CH}(\text{CH}_3)-\text{COOH}$	occurs in small quantities in blood and muscle fluid of man & animals also present in other organs & body fluids (3)	inhalation of mist causes coughing and irritation of mucous membranes (2)	not available (6)

<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
91	propyl mercaptan derivative		$\text{CH}_3\text{CH}_2\text{CH}_2\text{SO}^-$	no data available	no data available	not avail. (6)
93	ethyl mercaptan derivative	ethanethiol	$\text{CH}_3\text{CH}_2\text{SO}_2^-$	no data available	no data available	not avail.
93	phenol	hydroxy benzene		as a general disinfectant, either in solution or mixed with slaked lime, etc. for toilets, cesspools, floors, drains, etc. manuf of colorless resins, many medical and industrial organic cpds and dyes; as a reagent for chemical analysis (3)	Chronic poisoning with renal and hepatic damage may occur from industrial contact. Fatal poisoning may also occur by skin absorption. Ingestion of small amts may cause nausea, vomiting, circulatory collapse, paralysis, convulsions, coma, greenish or smoky colored urine and eventually death from respiratory failure (3)	5ppm (1)
95	methanesulfonic acid	methyl sulfonic acid		as catalyst in polymerization, alkylation and esterification reactions, as a solvent (3)	strong irritant (3)	
101	valeric acid	pentanoic acid	$\text{C}_4\text{H}_9\text{COOH}$	intermediate in perfumery (3)	no data available	not pertinent (5)

<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
105	butyl mercaptan derivative		$C_4H_9SO^-$	no data available	no data available	
107	propyl mercaptan derivative		$C_3H_7SO_2^-$	no data available	no data available	
107	cresol			disinfectants and fumigants, in photographic developers; also as a solvent (3)	oral or chronic percutaneous absorption may produce digestive disturbances, nervous disorders with faintness, vertigo, mental changes, skin eruptions, jaundice, general protoplasmic poisoning (3)	5ppm (5)
108	nicotiny alcohol	3-pyridine methanol		free alcohol is proposed as a solubilizer for riboflavin (3)	Therap cat: peripheral vasodilator; antilipemic (3)	
111	sorbic acid	2,4-hexadienoic acid		mold and yeast inhibitor. Fungistatic agent for foods, especially cheeses. In alkyd type coatings to improve gloss To improve milling characteristics of cold rubber (3)	no data available	
115	levulinic acid	4-oxopentanoic acid		in organic synthesis; in manuf of nylon, synthetic rubbers, plastics, medicinals (3)	no data available	

<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
115	fumaric acid	(E)-butenedioic acid	$\begin{array}{c} \text{HOOCCH} \\ \\ \text{HCCOOH} \end{array}$	substitute for tartaric acid in beverages and baking powders. As an antioxidant. Manuf polyhydric alcohols, synthetic resins. As mordant in dyeing (3)	Oral ingestion: 500 mg/day for a year is tolerated. Inhalation of dust may cause respiratory irritation (6)	not available (6)
115	maleic acid	(Z)-butenedioic acid		manuf of artificial resins, to retard rancidity of fats and oils; dyeing and finishing wool, cotton and silk (3)	strong irritant to nose, throat, eyes or skin (6)	not available (6)
115	caproic acid	hexanoic acid	$\text{CH}_3(\text{CH}_2)\text{COOH}$	manuf of esters for artificial flavors and of hexyl derivatives, especially hexylphenols, hexylresorcinol etc. (3)	no data available	not pertinent
121	butyl mercaptan derivative		$\text{C}_4\text{H}_9\text{SO}_2^-$	no data available	no data available	
121	ethyl sulfide			no data available	no data available	
121	benzoic acid	benzene carboxylic acid		preserving foods, fats, fruit juices alkaloidal solutions, etc. manuf benzoates and benzoyl cpds, dyes; as a mordant in calico printing, for curing tobacco (3)	Therap Cat: Pharmaceutical aid (antifungal agent) (3) mild irritant to skin, eyes and mucous membranes (6)	not pertinent (6)
121	dimethylphenol			intermediate in mfg of phenolic antioxidants; plastics & resins mfg; disinfectants mfg, insecticides & fungicides, rubber chemicals mfg, wetting agent, dyestuffs (3)	no data available	

<u>M/Z</u>	<u>COMPOUND</u>	<u>SYNONYM</u>	<u>STRUCTURE</u>	<u>USES</u>	<u>TOXICITY</u>	<u>TLV</u>
122	nitrosophenol	quinone oxime		no data available	can cause skin irritation, sensitization (3)	
122	picolinic acid	2-pyridine carboxylic acid		no data available	no data available	
123	propyl mercaptan derivative			no data available		
127	cyclohexane carboxylic acid			solubilizer for vulcanized rubber; clarifier for mineral oil, in insecticide formulations (3)	no data available	
129	heptanoic acid			no data available	no data available	
131	heptyl mercaptan		$C_7H_{15}S^-$	no data available	no data available	
135	toluic acid	methyl benzoic acid		no data available	no data available	
135	pentyl mercaptan derivative		$C_5H_{11}SO_2^-$	no data available	no data available	
135	phenylacetic acid			starting material in manuf synthetic perfumes (3)	no data available	
139	fluorobenzoic acid			no data available	no data available	
141	kojic acid	5-hydroxy-2(hydroxymethyl)-4H-pyran-4-one		converted to maltol and ethyl maltol, no data available flavor enhancing additives (3)		
143	caprylic acid	octanoic acid		an intermediate in manuf of esters used in perfumery; in manuf of dyes, etc. (3)	no data available	

M/Z	COMPOUND	SYNONYM	STRUCTURE	USES	TOXICITY	TLV
153	thiosalicylic acid			manuf of thioindigo dyes (3)		
157	pelargonic acid	nonanoic acid		manuf of lacquers and plastics (3)	strong irritant (3)	
167	dehydroacetic acid	3-acetyl-6-methyl-2H-pyran-2,4(3H)-dione		in organic sythesis; as plasticizer, compatible with nitrocellulose, polystyrene, methacrylate, vinylite resins, (3)	causes impaired kidney function, large doses can cause vomiting, ataxia, convulsions (3)	not available
169	dithiosalicylic acid					
171	toluenesulfonic acid	methylbenzene sulfonic acid		in dye chemistry. Also in manuf of oral antidiabetic drugs (3)	highly irritating to skin, mucous membranes (6)	not available
171	capric acid	decanoic acid	$\text{CH}_3(\text{CH}_2)_8\text{COOH}$	manuf of esters for artificial fruit flavors and perfumes; as an intermediate in other chemical synthesis (3)		
183	diazobenzene sulfonic acid			in manuf of azo dyes (3)		
185	iodoacetic acid					

Abbreviations:

T.L.V. = Threshold Limit Values

P.O.L. = Provisional Operational Limit

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